



## **Technical Note**

**TN – KLH 2/2002**

### **Fire Benchmark #2**

#### **Part 1:**

#### **Fire in a large Hall**

**CFX and COCOSYS**

**Preliminary Results**

**- DRAFT VERSION-**

**W. Klein-Heßling**

**April 2002, Draft Version**



## **Content**

<b>1</b>	<b>Introduction.....</b>	<b>1</b>
<b>2</b>	<b>Nodalisation and used Models.....</b>	<b>1</b>
<b>3</b>	<b>Preliminary results .....</b>	<b>4</b>
<b>3.1</b>	<b>Case 1 .....</b>	<b>4</b>
<b>3.2</b>	<b>Case 2 .....</b>	<b>11</b>
<b>3.3</b>	<b>Case 3 .....</b>	<b>18</b>
<b>3.4</b>	<b>Comparison between the cases .....</b>	<b>23</b>
<b>4</b>	<b>Conclusions - Next steps.....</b>	<b>25</b>

## List of figures

Fig. 2-1	COOSYS Nodalisation: side view .....	2
Fig. 2-2	COOSYS Nodalisation: top view.....	3
Fig. 2-3	COOSYS Nodalisation.....	3
Fig. 3-1	Case1: temperatures at lower part of tree 1 .....	5
Fig. 3-2	Case1 : tempertures at upper part of tree 1 .....	6
Fig. 3-3	Case1: temperatures at lower part of tree 2 .....	6
Fig. 3-4	Case1: temperatures at upper part of tree 2 .....	7
Fig. 3-5	Case1: Temperatures at lower part of tree 3.....	7
Fig. 3-6	Case1: Temperatures at upper part of tree 3 .....	8
Fig. 3-7	Case1: Comparison between the different variations of calculation.....	8
Fig. 3-8	Case1: Plume temperatures.....	9
Fig. 3-9	Visualisation of the fire plume (temperature) in COOSYS .....	9
Fig. 3-10	Visualisation of the fire plume (temperature) in CFX.....	10
Fig. 3-11	Case1: Interface height .....	10
Fig. 3-12	Case1: Upper layer temperature .....	11
Fig. 3-13	Case2: Temperatures at the lower part of tree 1.....	12
Fig. 3-14	Case2: Temperatures at the upper part of tree 1 .....	13
Fig. 3-15	Case2: Temperatures at the lower part of tree 2.....	13
Fig. 3-16	Case2: Temperatures at the upper part of tree 2 .....	14
Fig. 3-17	Case2: Temperatures at the lower part of tree 3.....	14
Fig. 3-18	Case2: Temperatures at the upper part of tree 3 .....	15
Fig. 3-19	Case2: Temperatures inside the plume.....	15
Fig. 3-20	Case2: Heat flow to the wall structures .....	16
Fig. 3-21	Case2: Calculated mass flow rates through the infiltrations.....	16
Fig. 3-22	Interface height in case 2 .....	17
Fig. 3-23	Upper layer temperature in case 2 .....	17
Fig. 3-24	Case3: Temperatures at lower part of tree 1.....	18
Fig. 3-25	Case 3: Temperature at upper part of tree 1 .....	19
Fig. 3-26	Case 3: Temperature at lower part of tree 2.....	19
Fig. 3-27	Case 3: Temperature at upper part of tree 2.....	20
Fig. 3-28	Case 3: Temperature at lower part of tree 3.....	20
Fig. 3-29	Case 3: Temperature at upper part of tree 3.....	21
Fig. 3-30	Case 3: Plume temperatures.....	21
Fig. 3-31	Case 3: Injected and burned heptan mass.....	22

Fig. 3-32 Case 3: Interface height .....	22
Fig. 3-33 Upper layer temperature.....	23
Fig. 3-34 Calculated heat release rates for the 3 cases .....	24
Fig. 3-35 Comparison of the measured and calculated temperatures at T1.10.....	24
Fig. 3-36 Comparison of CFX and COCOSYS for all cases.....	25



## **1           Introduction**

In the frame of the "International Collaborative Project to Evaluate Fire Models for Nuclear Power Plant Applications" a second benchmark exercise have been performed. In this exercise different pool fire experiments in a large hall have been investigated. In this technical note first results of performed COCOSYS calculations and some CFX preliminary results are discussed.

COCOSYS is a so-called lumped-parameter code. To simulate the local conditions (natural convection, temperature stratification) the fire hall is divided into a quite high number of control volumes. The main idea is to have for each temperature measurement a separate control volume and to have separate control volumes around the fire plume, the ventilation system and the doors.

CFX is a CFD program. The k- $\epsilon$  model has been used for the simulation of turbulence. For the reaction the eddy-break-up model has been used. CFX has a separate radiation model RAD3D to consider the heat distribution of the flame.

**The CFX calculations have been performed by M. Heitsch. The results of COCOSYS and CFX are preliminary.**

## **2           Nodalisation and used Models**

For COCOSYS a detailed subdivision of the fire hall has been used. Fig. 2-1 to Fig. 2-3 show the nodalisation of the fire hall. With this subdivision nearly all temperature measurements have a separate control volume. There a direct comparison between experimental measurements and calculated results is possible. The total number of control volumes is 543.

The control volumes above the pool have an area of 6 m<sup>2</sup>. This leads to some averaging of the temperatures in the fire plume. COCOSYS itself has no specific plume model.

The flow between the control volumes is mainly buoyancy driven. A momentum balance is not calculated.

For the calculations the given pyrolysis rates are used. In the first calculation the calculated temperature has been calculated to high. Therefore the reaction rate above the pool has been reduced by an additional factor FEFF of 60%. The remaining unburned heptan may be burned in upward direction. 20% of the reaction heat is distributed by radiation to the wall structures. The view factors used have been calculated by the new grid generator for COCOSYS. For the heat exchange between the walls and atmosphere the specified heat transfer coefficient and the COCOSYS heat transfer models for free convection have been used, respectively.

In the CFX calculations following standard models have been used:

- for the simulation of combustion the eddy-break-up model (for each cell)
- k-e model for turbulence
- the radiation is simulated by RAD3D
- the Magnussen-Model for the simulation of soot behavior

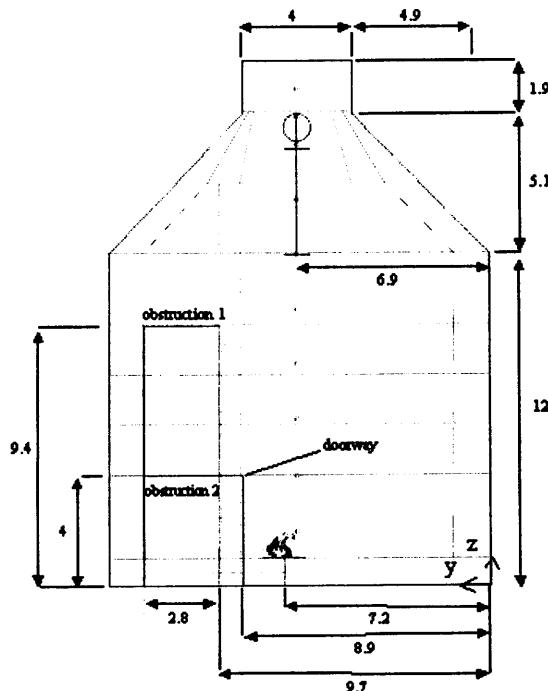


Fig. 2-1 COCOSYS Nodalisation: side view

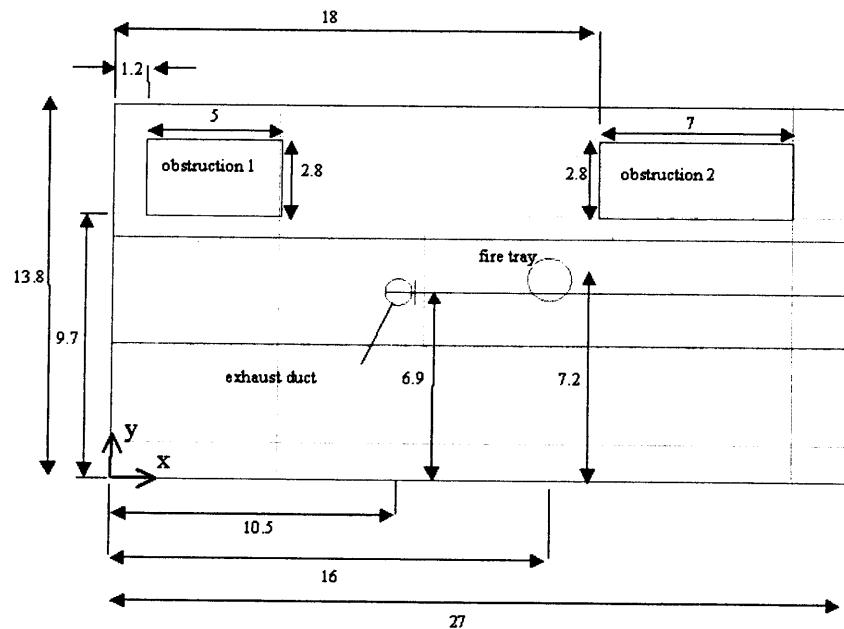


Fig. 2-2 COCOSYS Nodalisation: top view

**Fire benchmark #2  
COCOSYS nodalisation**

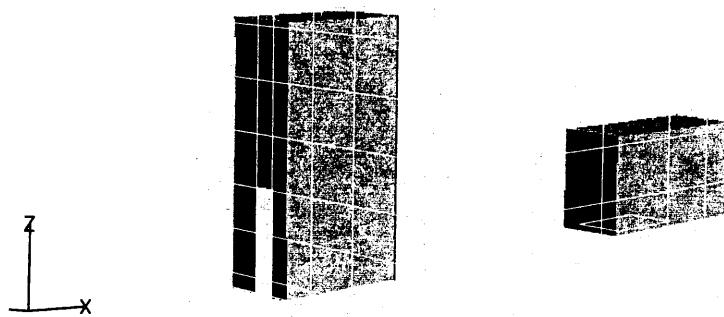


Fig. 2-3 COCOSYS Nodalisation

### 3 Preliminary results

In the following sections the preliminary results will be discussed. The figures show the actual status of the COCOSYS results for the three specified cases of part 1 and some CFX results for comparison reason.

#### 3.1 Case 1

Fig. 3-1 to Fig. 3-6 show the comparison between the optimal COCOSYS calculation and the measurements at the 3 temperature trees. The quality of the results is quite well. The stratification of the temperatures at the upper measurement points is calculated somewhat too high. The main reason is the missing momentum balance in the COCOSYS calculation. The mass flow between the control volumes is mainly induced by the buoyancy leading to stratified results.

It has been pointed out, that the reaction efficiency is adjusted to the temperatures. Unfortunately there is no additional possibility to check this modeling assumption, like concentration measurements or measurement data of the temperature decrease after the burning process.

Fig. 3-7 shows the temperatures at T1.6 and T1.10 for the different variations of COCOSYS calculations and the CFX results. The CFX result is similar to the *COCfull* case of COCOSYS. Both calculation assume a full reaction of the heptan. The differences between the green (COCbase) and red (COCopt) curve results from the different assumptions for the heat transfer to the boundary and the infiltration. In the COCopt case the COCOSYS heat transfer models for free convection are used, the walls are handled non-adiabatic on the outer side and a half of the infiltration from the upper position are shifted to the top of the roof. Assuming the full reaction the calculated temperatures are about 50 K too high. The influence of the different assumptions for heat transfer and infiltration leads to a temperature decreasing of about 15 to 20 K. Therefore the main effect results from the decreasing of the reaction efficiency.

The beginning of the temperature decrease after the burning process shows the right behavior. But the time period is too short, to conclude that the calculated heat loss into the walls and through the infiltration is simulated correctly.

Fig. 3-8 presents the comparison of the plume temperatures TG1 and TG2. COCOSYS has no specific plume model. As already mentioned the plume is simulated of a column of control volumes above the pool. The area of these volumes is 6 m<sup>2</sup>. This lead to an averaging of the calculated temperatures. In the CFX calculation the temperatures are much higher and the behavior seems to be more realistic, also the temperature level is somewhat to high. A three-dimensional impression of the fire plume can be drawn from Fig. 3-9 for COCOSYS and Fig. 3-10 for CFX. Both figures show the temperature distribution in the middle yz-plane.

In the following figures the average values are presented. These have been calculated according the formulas specified in the benchmark description. Although the correspondence between the measured and calculated temperatures are quite well, the calculated interface height is too low (red curve).

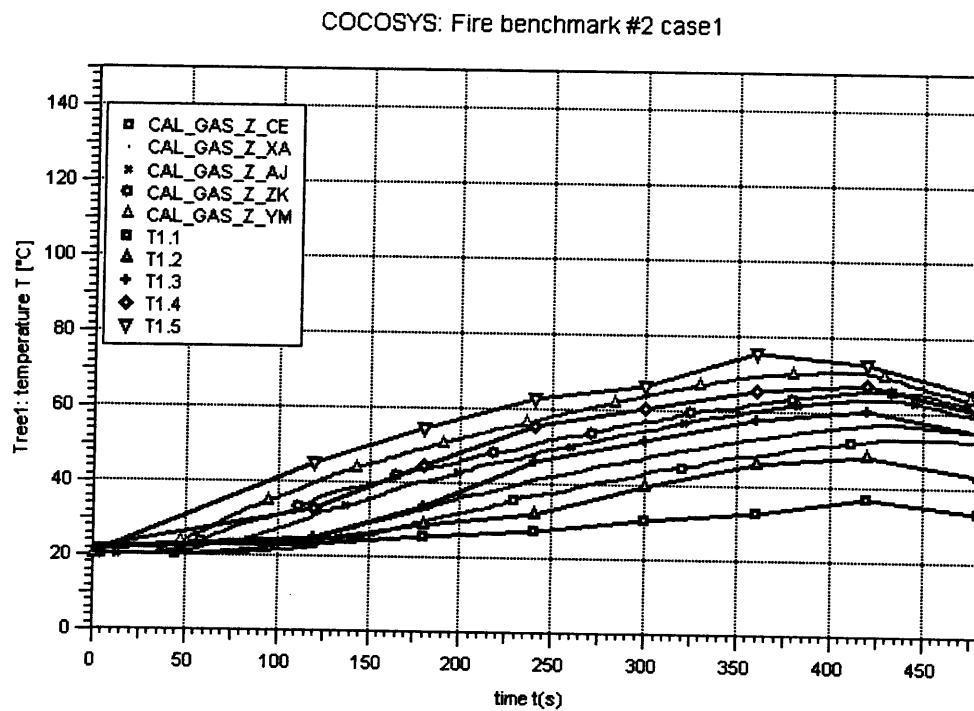


Fig. 3-1 Case1: temperatures at lower part of tree 1

COCOSYS: Fire benchmark #2 case1

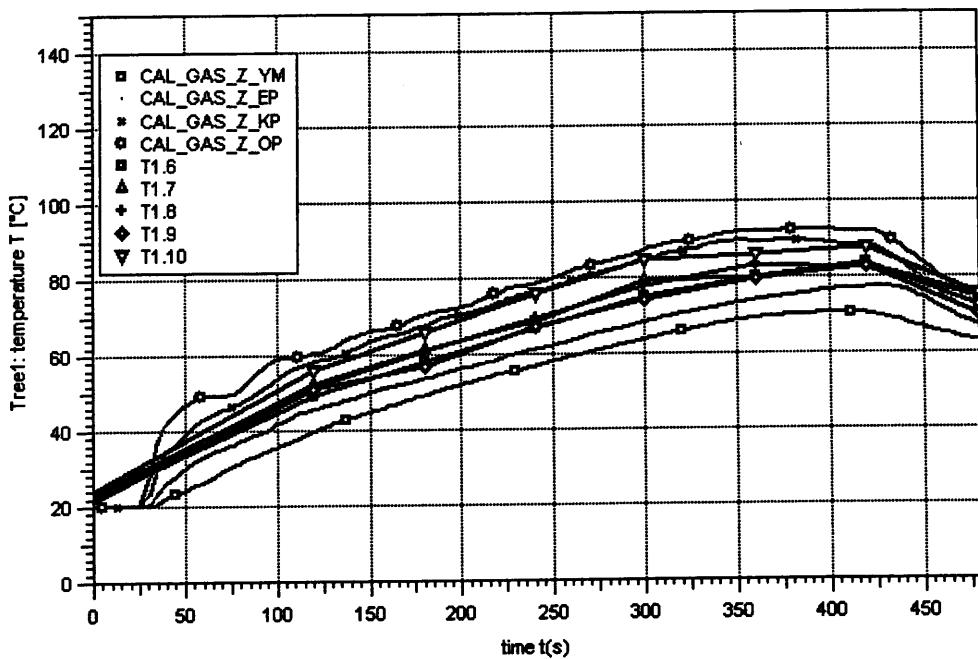


Fig. 3-2 Case1 : tempertures at upper part of tree 1

COCOSYS: Fire benchmark #2 case1

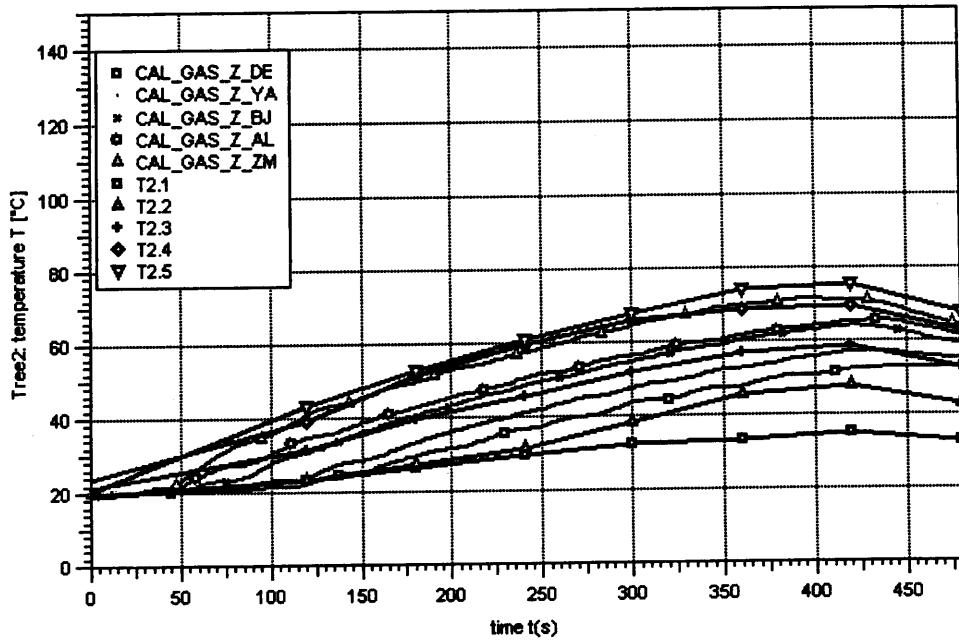


Fig. 3-3 Case1: temperatures at lower part of tree 2

COCOSYS: Fire benchmark #2 case1

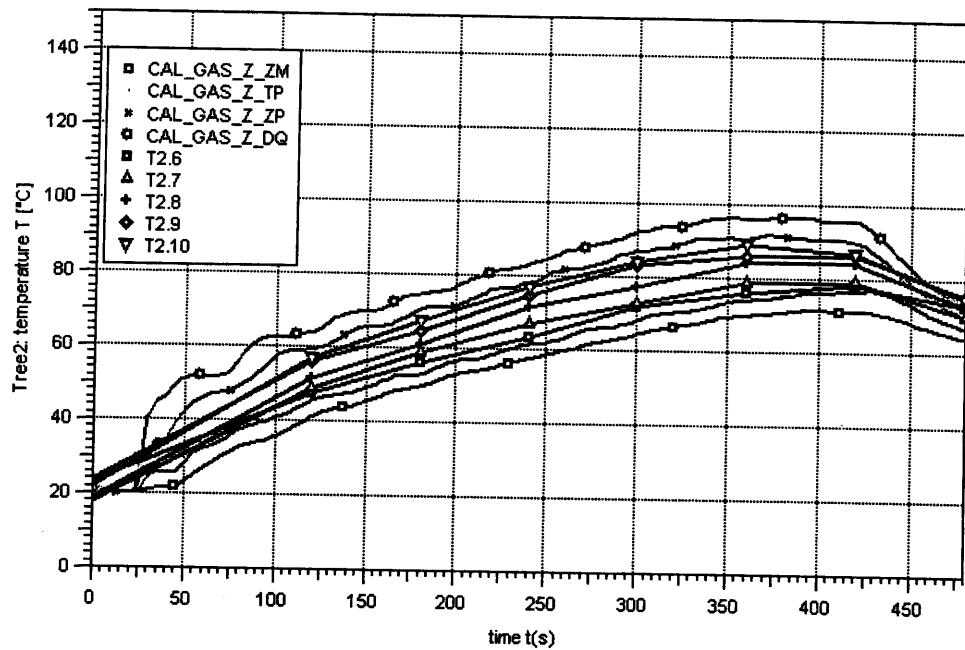


Fig. 3-4 Case1: temperatures at upper part of tree 2

COCOSYS: Fire benchmark #2 case1

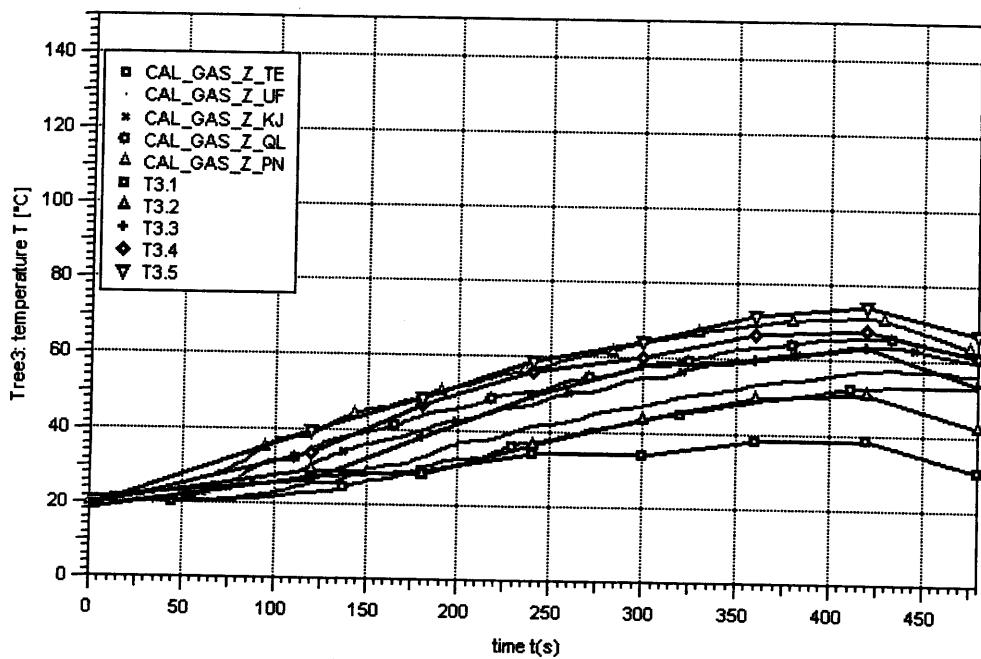


Fig. 3-5 Case1: Temperatures at lower part of tree 3

COCOSYS: Fire benchmark #2 case1

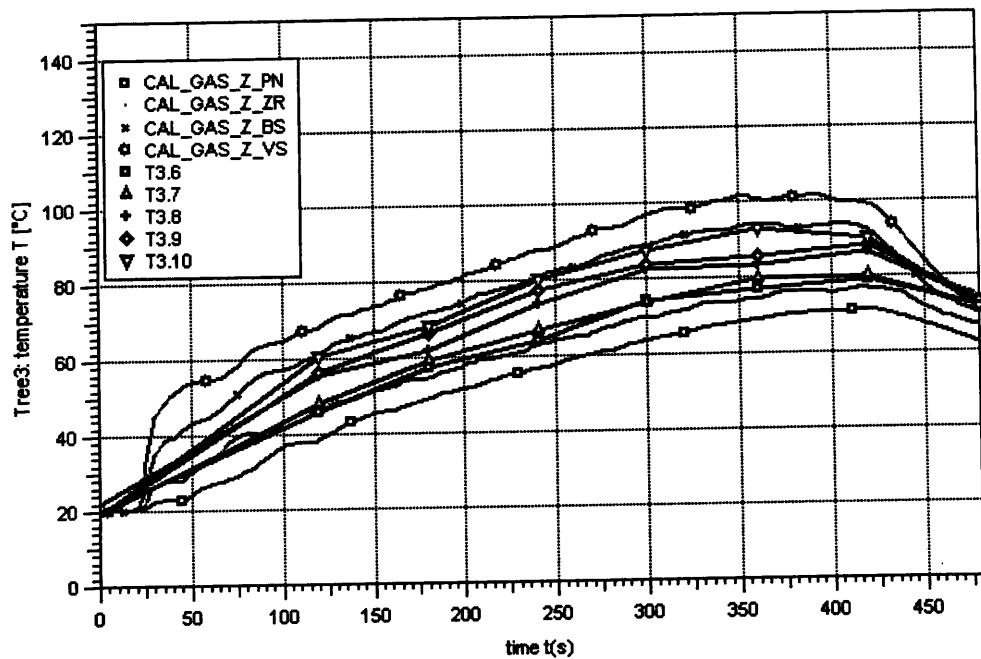


Fig. 3-6 Case1: Temperatures at upper part of tree 3

COCOSYS: Fire benchmark #2 case1

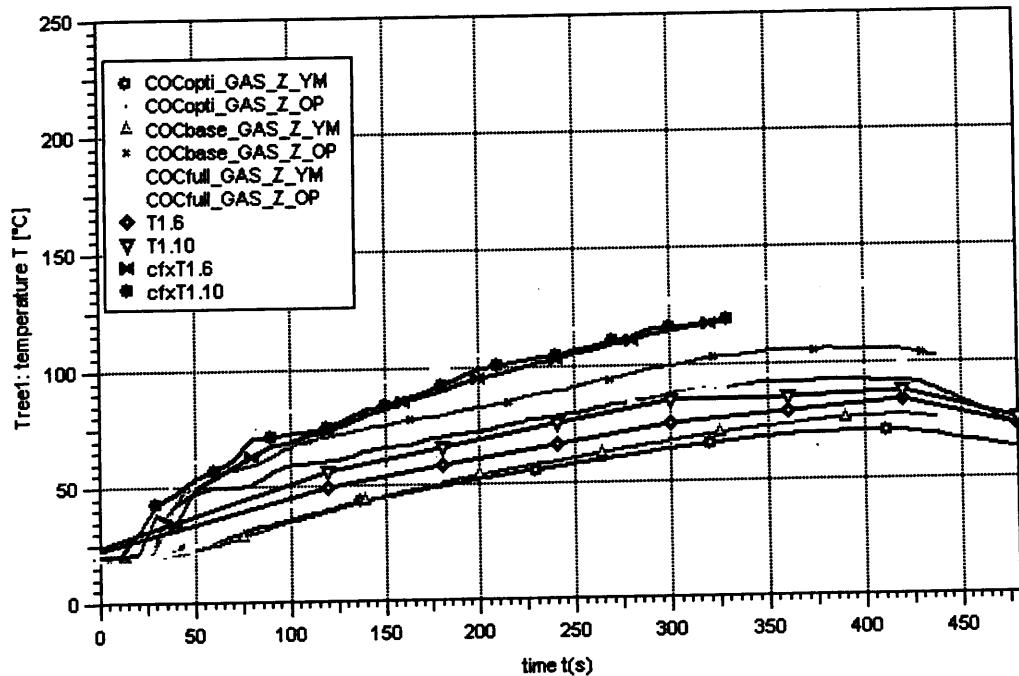


Fig. 3-7 Case1: Comparison between the different variations of calculation

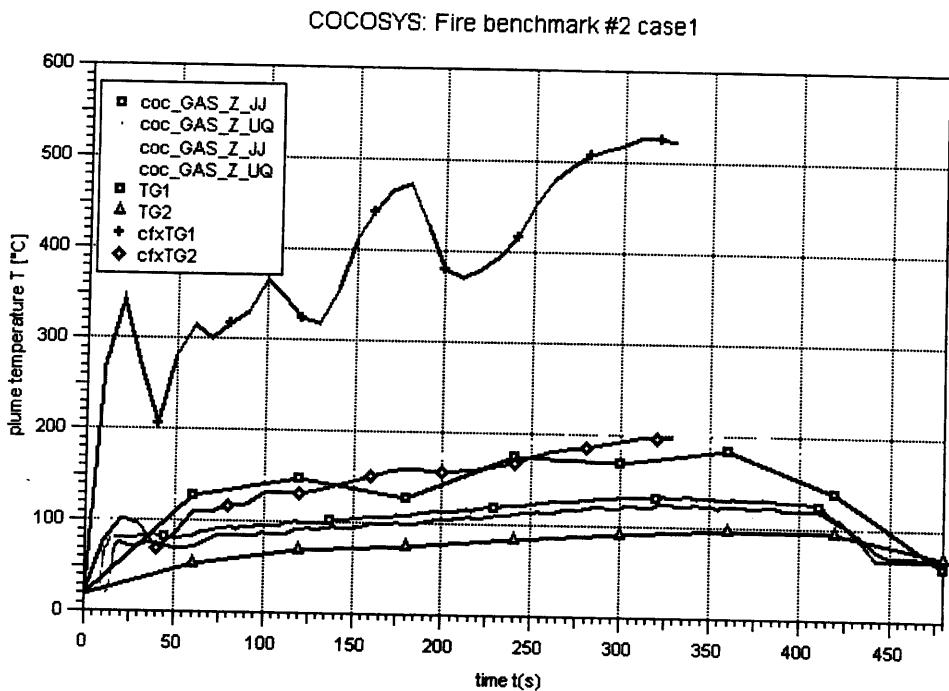


Fig. 3-8 Case1: Plume temperatures

**Fire Benchmark #2 case 1**  
COCOSYS calculation

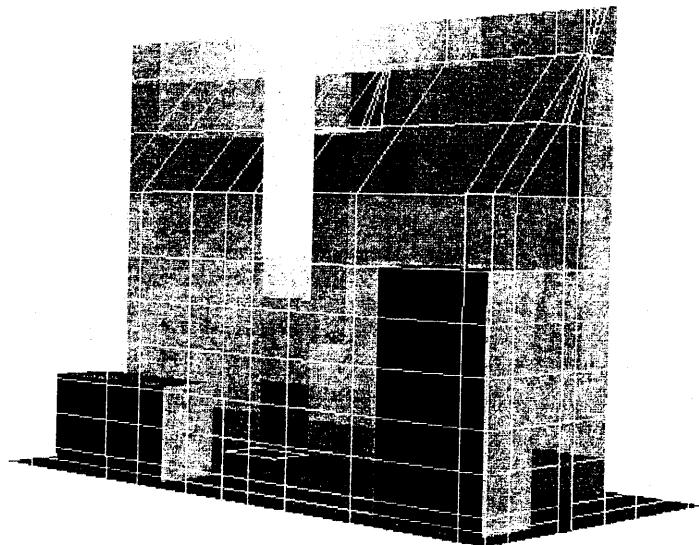


Fig. 3-9 Visualisation of the fire plume (temperature) in COCOSYS

**Fire Benchmark #2 part 1**  
CFX calculation case1

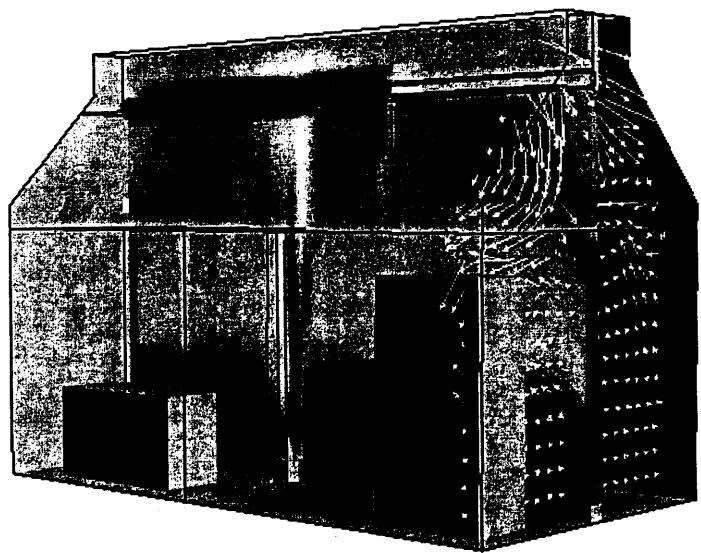


Fig. 3-10 Visualisation of the fire plume (temperature) in CFX

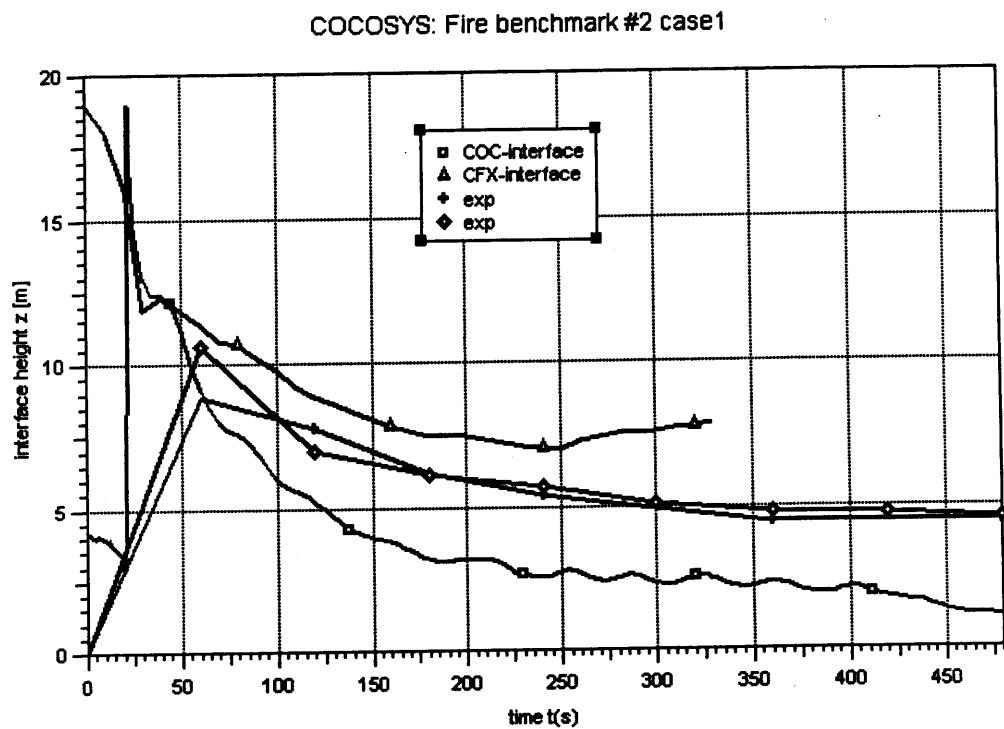


Fig. 3-11 Case1: Interface height

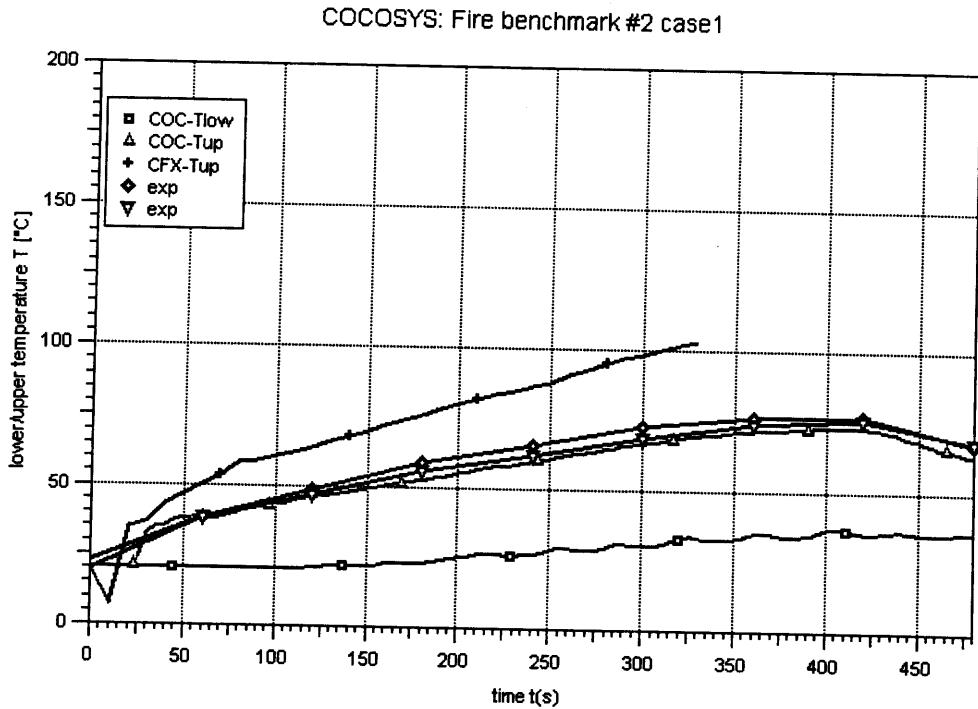


Fig. 3-12 Case1: Upper layer temperature

### 3.2 Case 2

Similar to case 1 COCOSYS simulates the temperatures quite well. The Fig. 3-13 to Fig. 3-18 show the comparison between the calculation and the measurement for the 3 measurement trees. As for the case 1 the calculated temperature stratification is calculated somewhat to strong. A similar behavior is also found for the calculated plume temperatures. Fig. 3-19 shows the different values of plume temperature for a calculation with a complete reaction of heptan over the pool surface (*COCfull*) and the optimal case with a 60% reaction efficiency. Because only the temperatures can be compared, an additional consistency check is not possible (for example for  $\text{CO}_2$  concentration).

Fig. 3-20 presents the comparison of the heat loss to the wall structures for different calculated variations. The red curve corresponds to the optimal COCOSYS case. In the base calculation of COCOSYS (*COCbase*) the infiltration, heat transfer conditions are set according the benchmark specification. The heat loss calculated in the CFX calculations is lower. This is a reason for the higher calculated temperatures too.

The mass flow rate through the infiltration depends strongly on the specified boundary conditions. Fig. 3-21 presents the comparison between the three COCOSYS calculations. In the first calculation (*COCfull*) all environmental control volumes are started with a total pressure of 1.013 bar. Because the total pressure in the roof part of the fire hall is smaller a convection loop in the wrong direction (from upper to the lower infiltration) starts. In the calculations *COCbase* and *COCopt* all mass flows are positive (from inside to outside) during the heat up phase. Later at about 150s a convection loop in the right direction starts. The differences between the red and green curves show the effect of the moved upper infiltration to the top of the hall roof.

Fig. 3-22 and Fig. 3-23 show the average values for the interface height and upper layer temperature. Also the correspondence between calculated and measured temperatures looks quite well, the calculated interface layer height is somewhat lower.

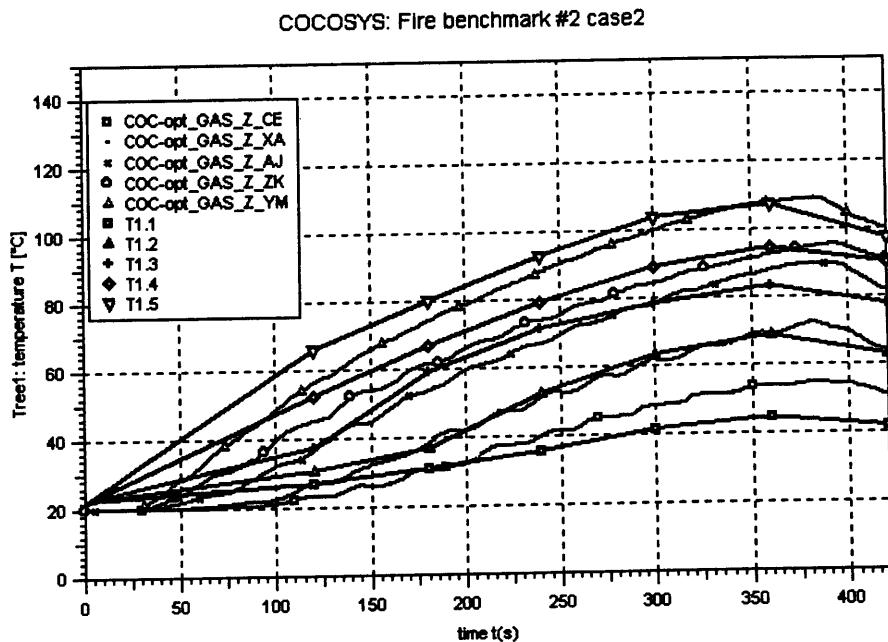


Fig. 3-13 Case2: Temperatures at the lower part of tree 1

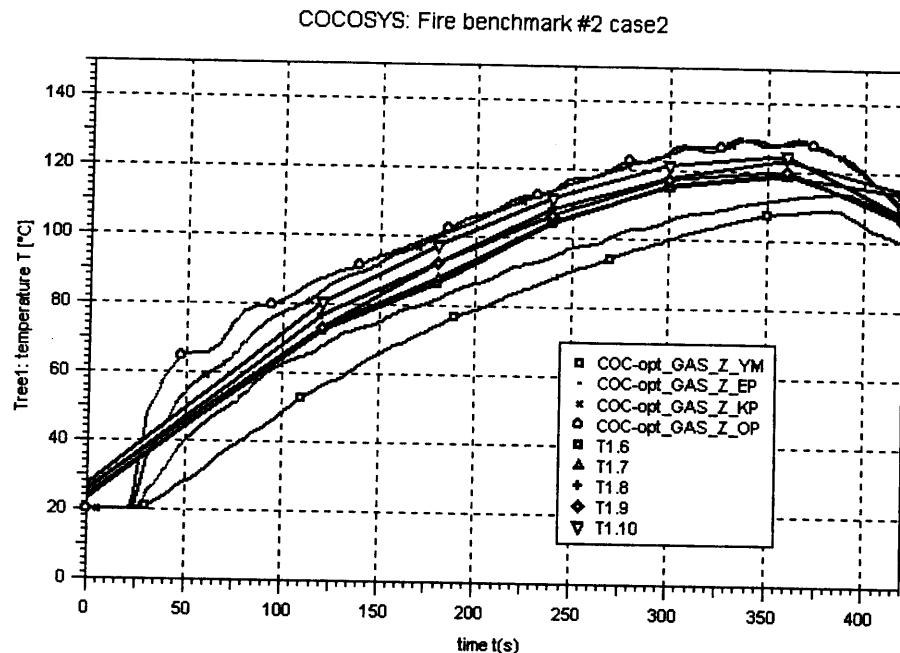


Fig. 3-14 Case2: Temperatures at the upper part of tree 1

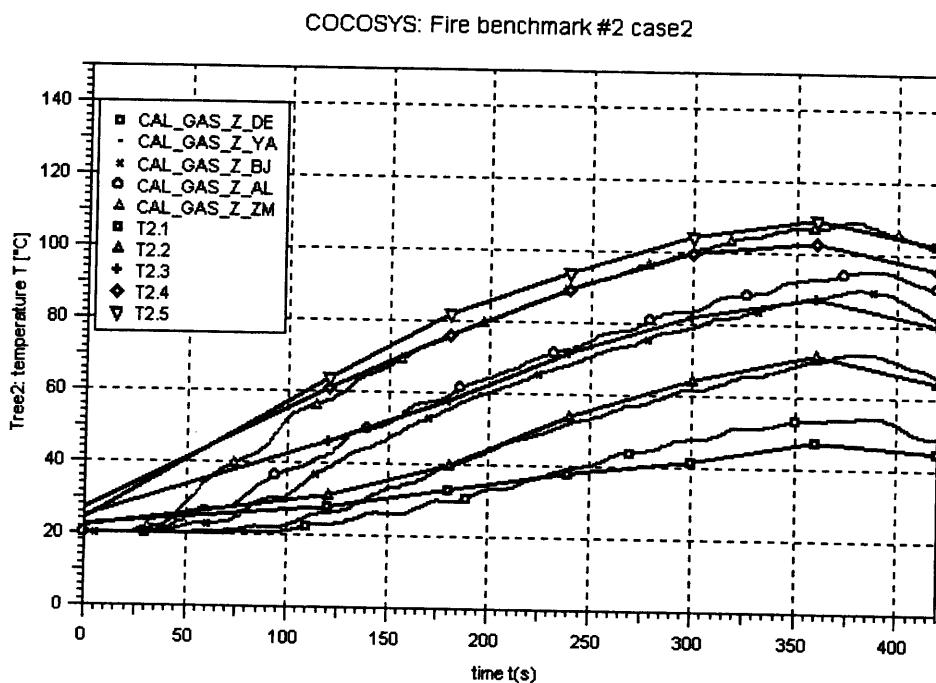


Fig. 3-15 Case2: Temperatures at the lower part of tree 2

COCOSYS: Fire benchmark #2 case2

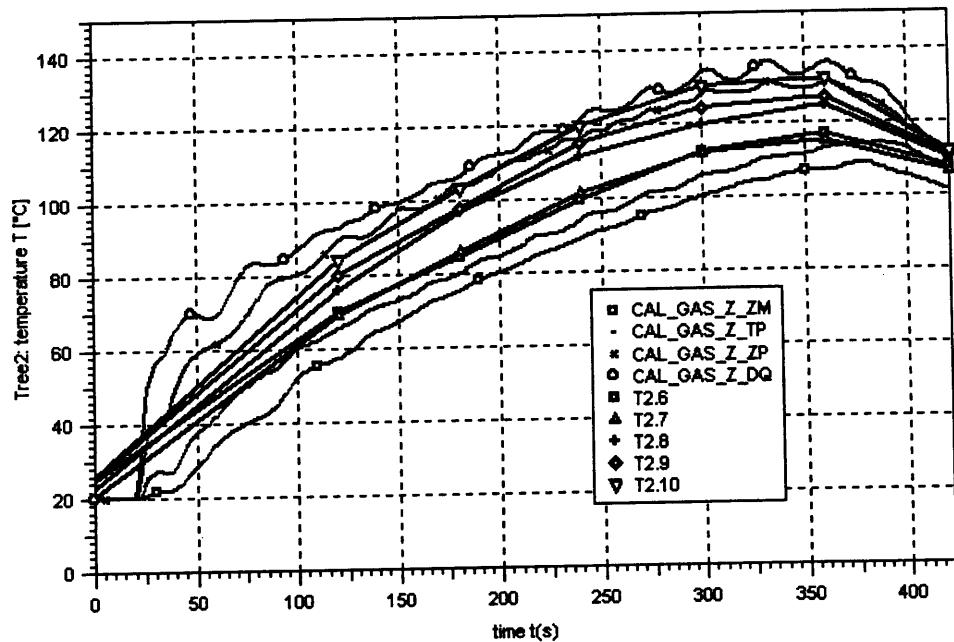


Fig. 3-16 Case2: Temperatures at the upper part of tree 2

COCOSYS: Fire benchmark #2 case2

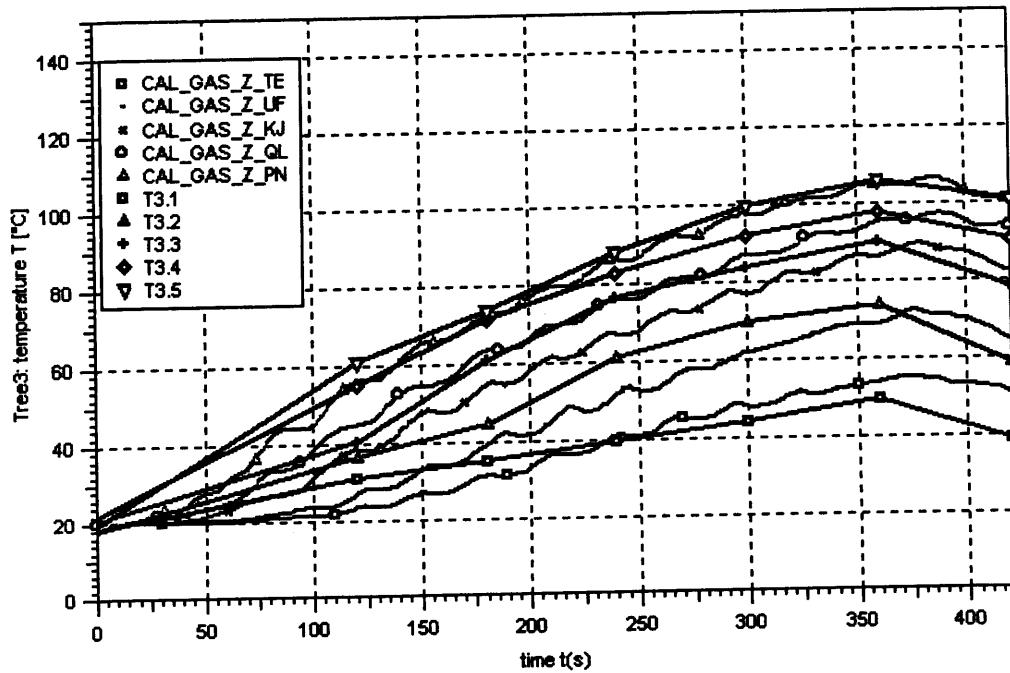


Fig. 3-17 Case2: Temperatures at the lower part of tree 3

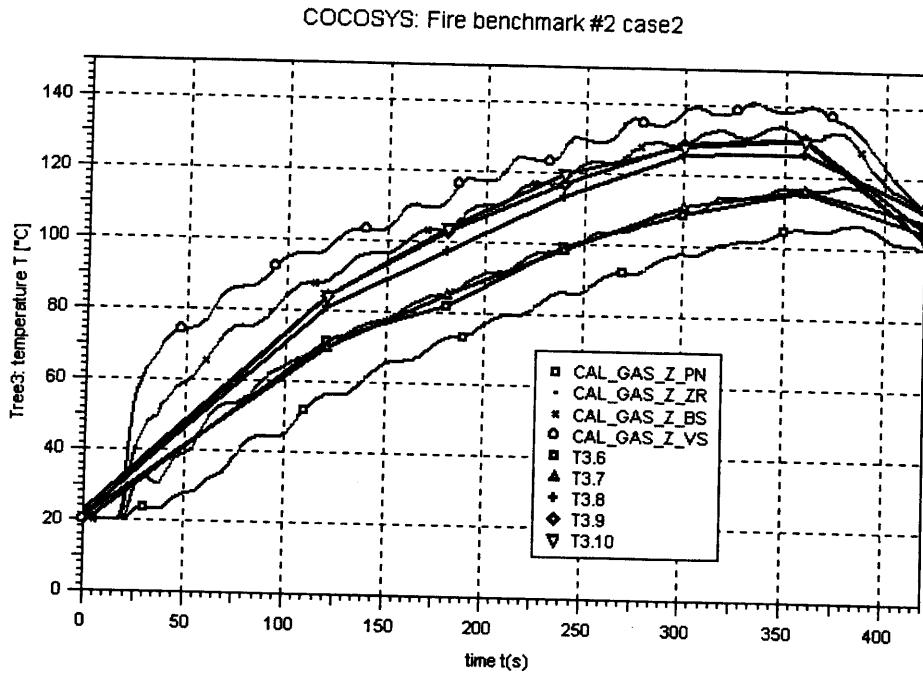


Fig. 3-18 Case2: Temperatures at the upper part of tree 3

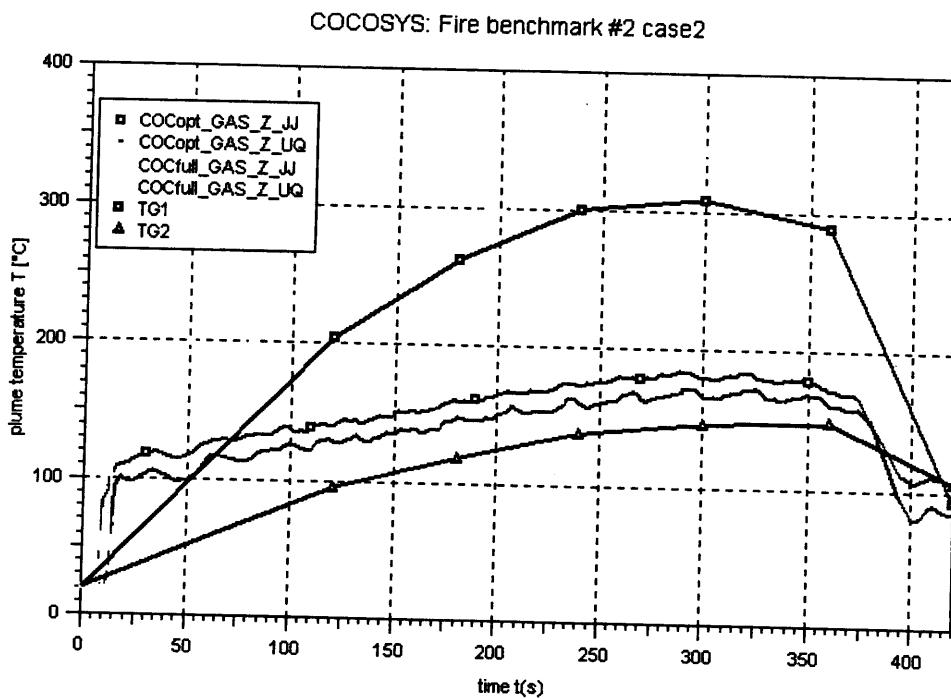


Fig. 3-19 Case2: Temperatures inside the plume

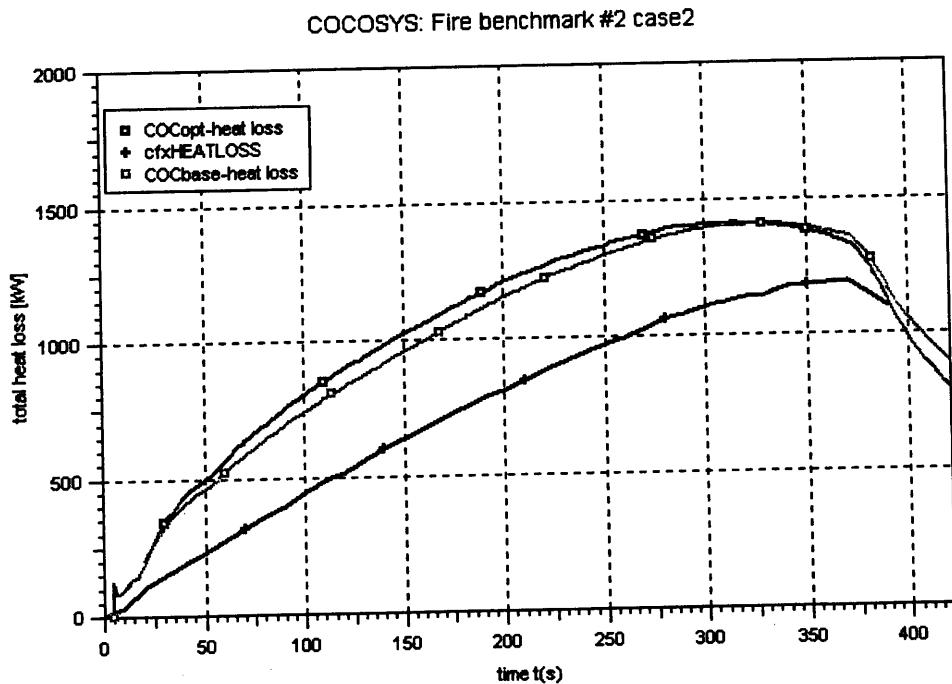


Fig. 3-20 Case2: Heat flow to the wall structures

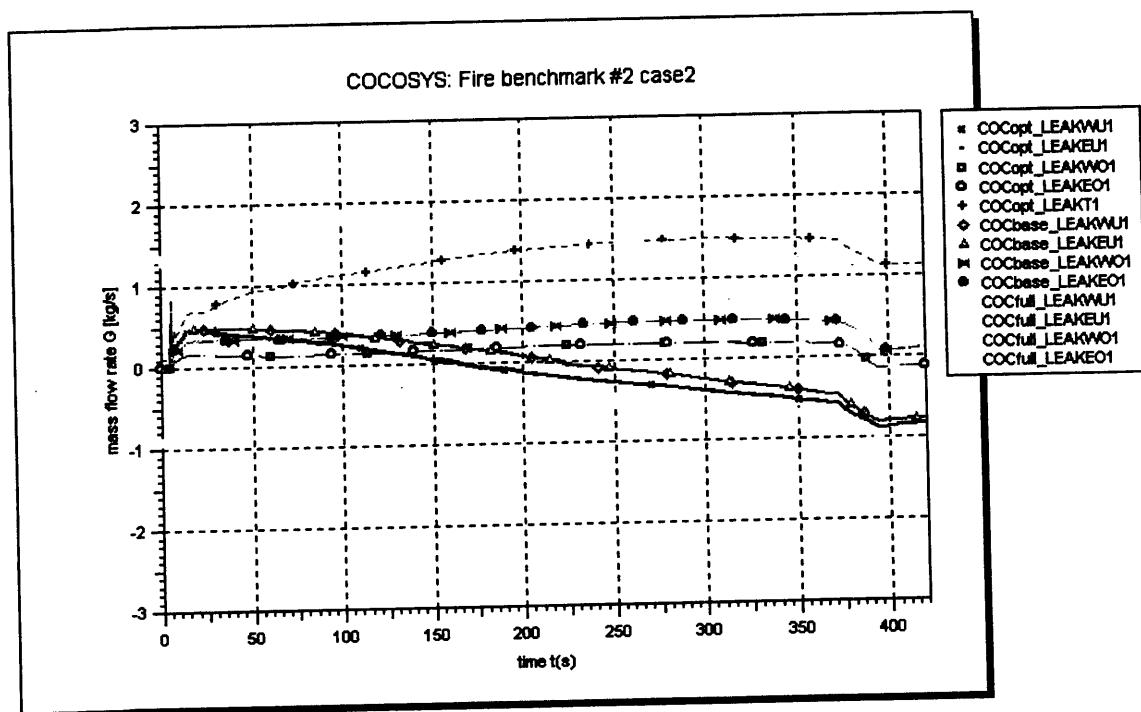


Fig. 3-21 Case2: Calculated mass flow rates through the infiltrations

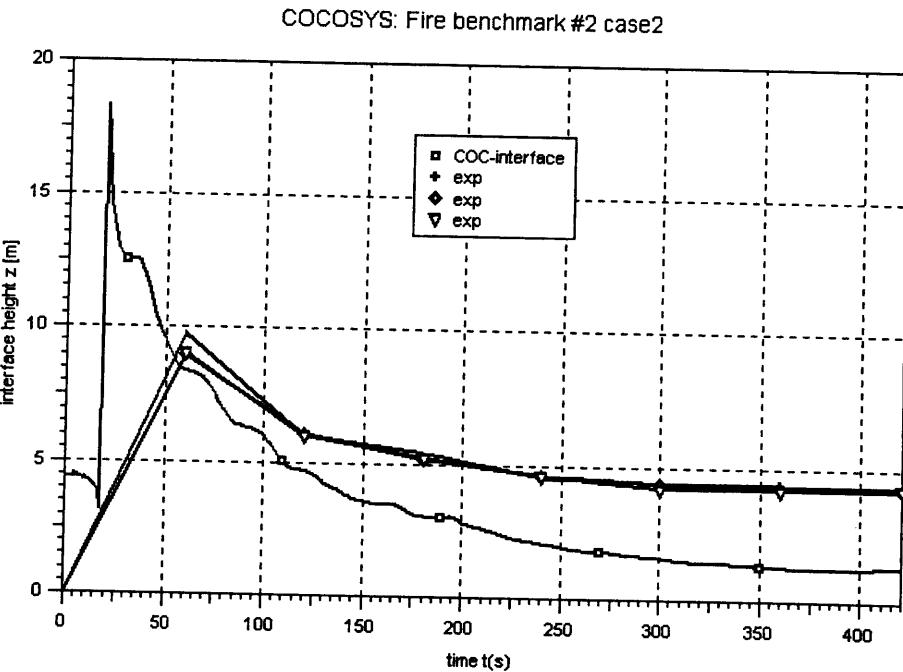


Fig. 3-22 Interface height in case 2

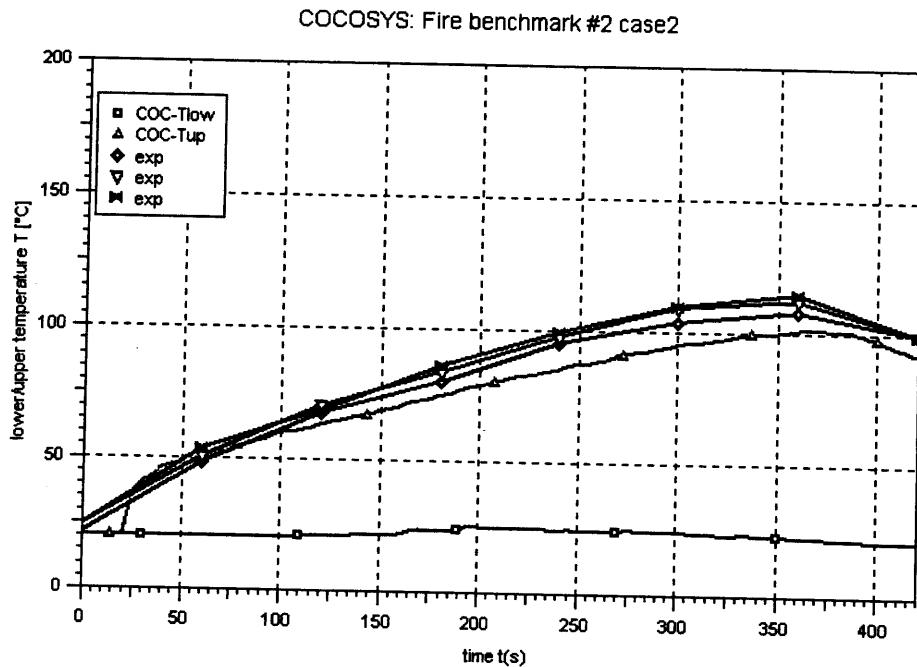


Fig. 3-23 Upper layer temperature in case 2

### 3.3 Case 3

Although the ventilation system has been used and the doors are open in case 3, the behavior is very similar to case 1 and 2. Fig. 3-24 to Fig. 3-30 show the results of the optimal COCOSYS calculation compared with the experimental measurements.

Fig. 3-31 presents the injected and burned mass of heptan. About 30% of the heptan mass remains unburned. This value is compared to the value specified in the benchmark description relatively high.

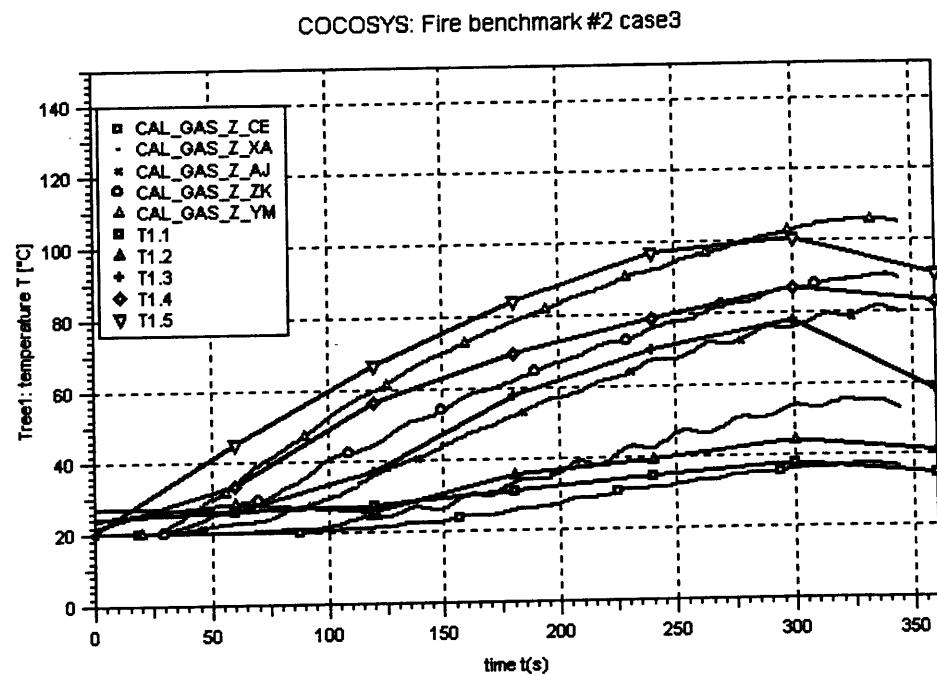


Fig. 3-24 Case3: Temperatures at lower part of tree 1

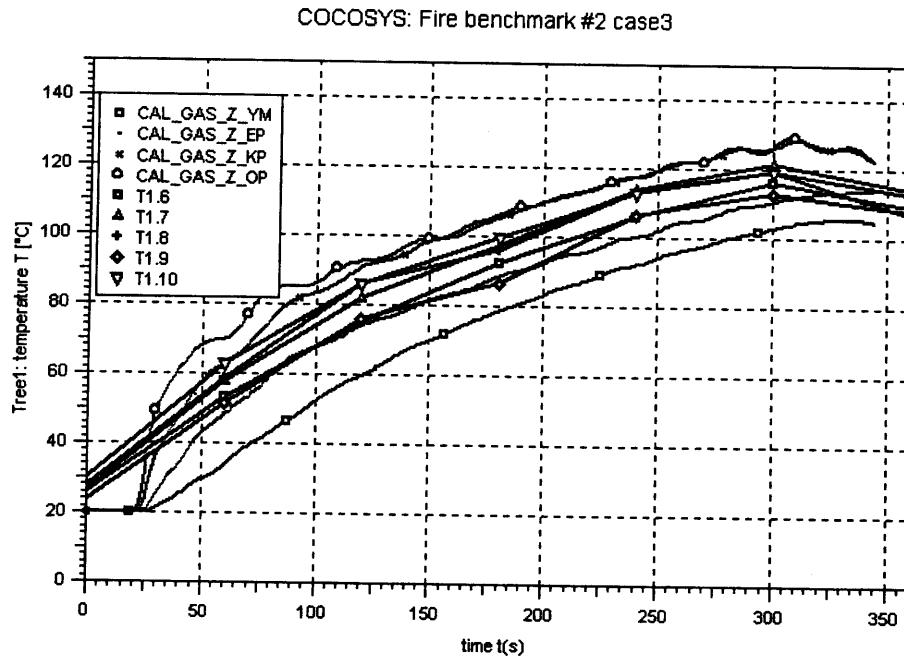


Fig. 3-25 Case 3: Temperature at upper part of tree 1

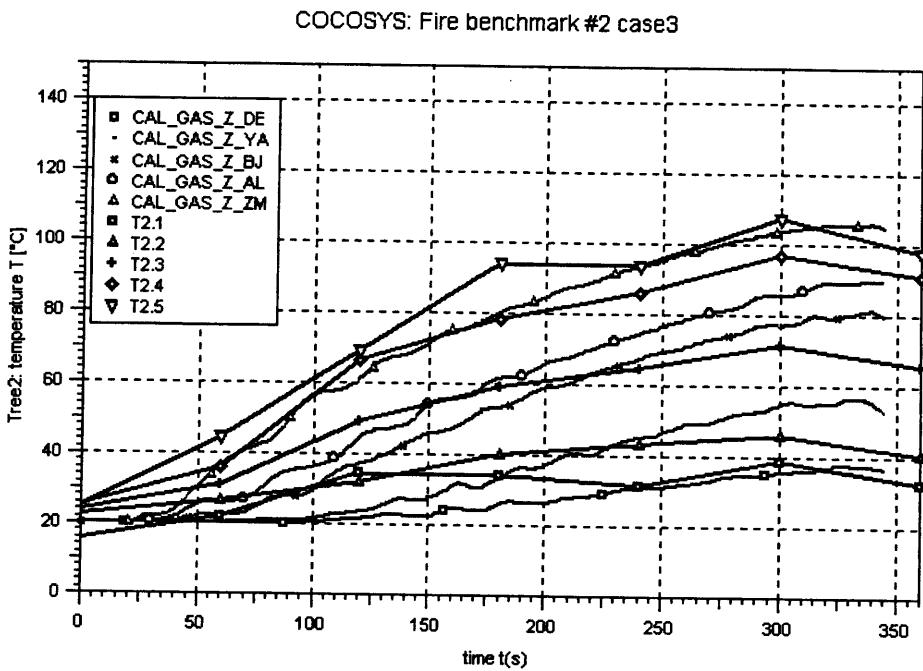


Fig. 3-26 Case 3: Temperature at lower part of tree 2

COCOSYS: Fire benchmark #2 case3

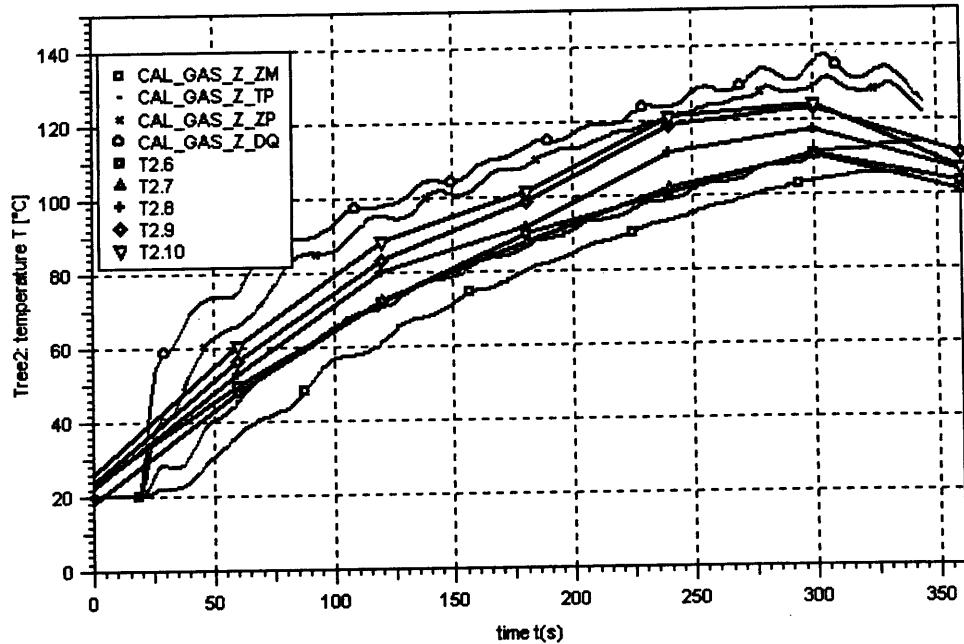


Fig. 3-27 Case 3: Temperature at upper part of tree 2

COCOSYS: Fire benchmark #2 case3

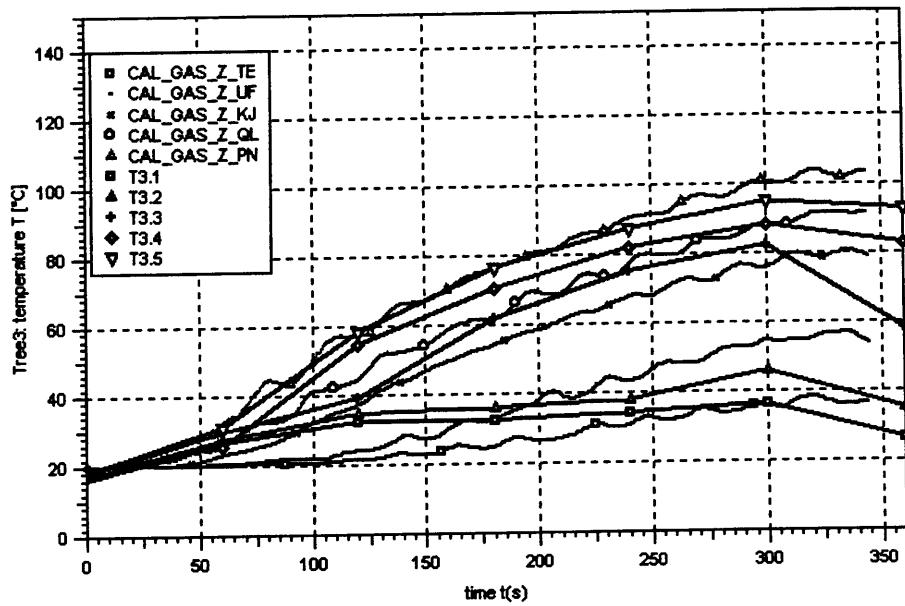


Fig. 3-28 Case 3: Temperature at lower part of tree 3

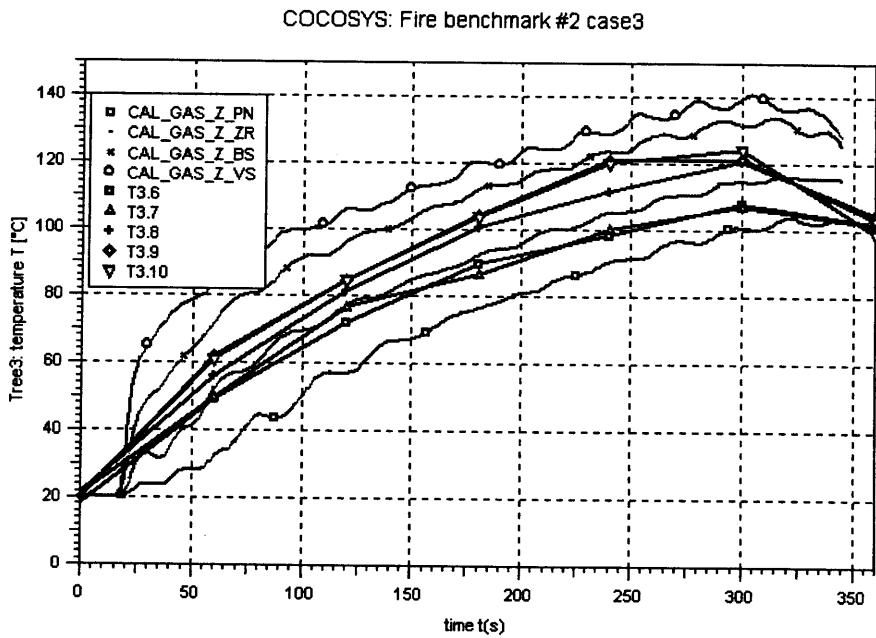


Fig. 3-29 Case 3: Temperature at upper part of tree 3

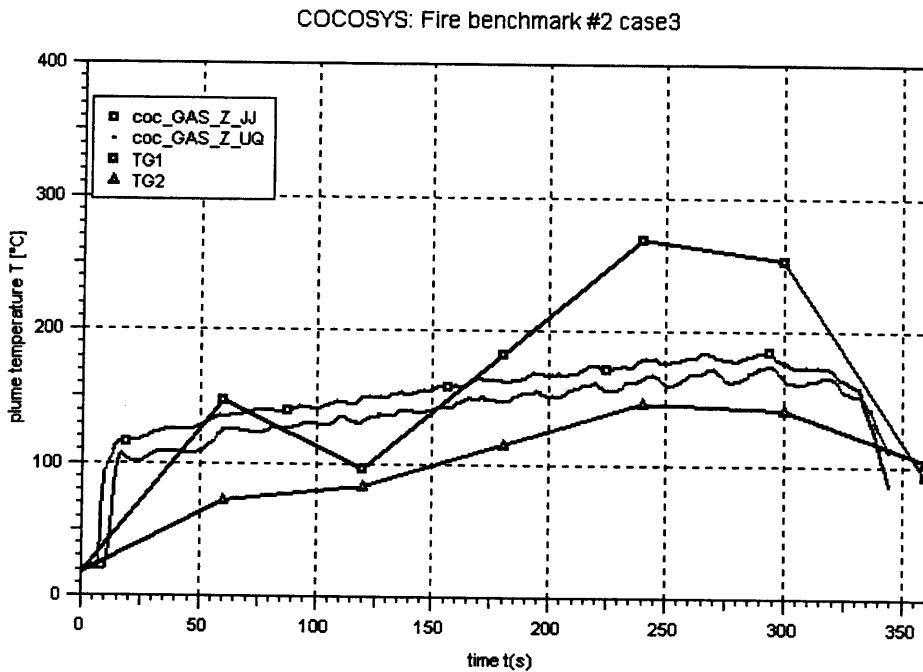


Fig. 3-30 Case 3: Plume temperatures

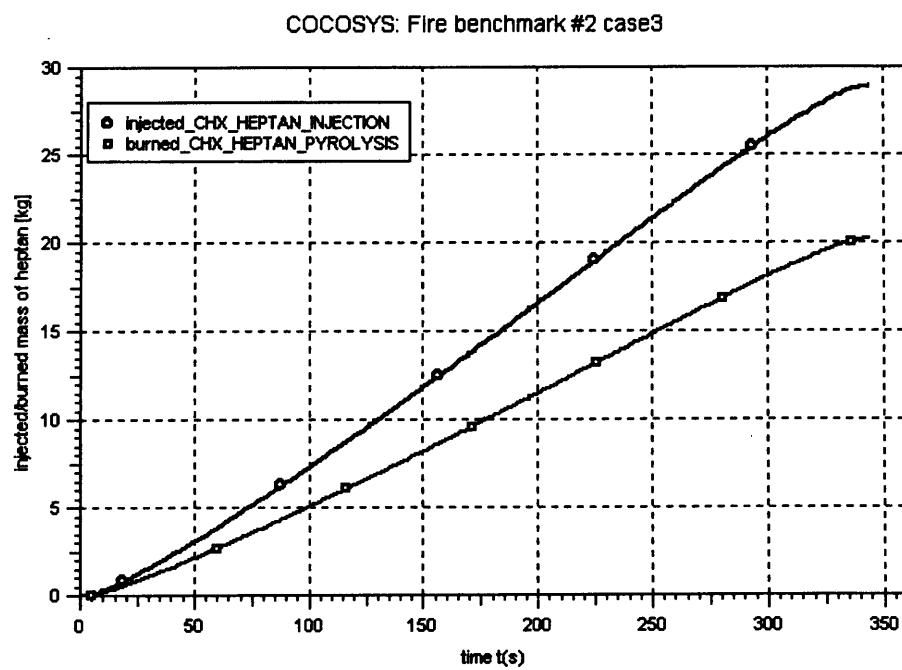


Fig. 3-31 Case 3: Injected and burned heptan mass

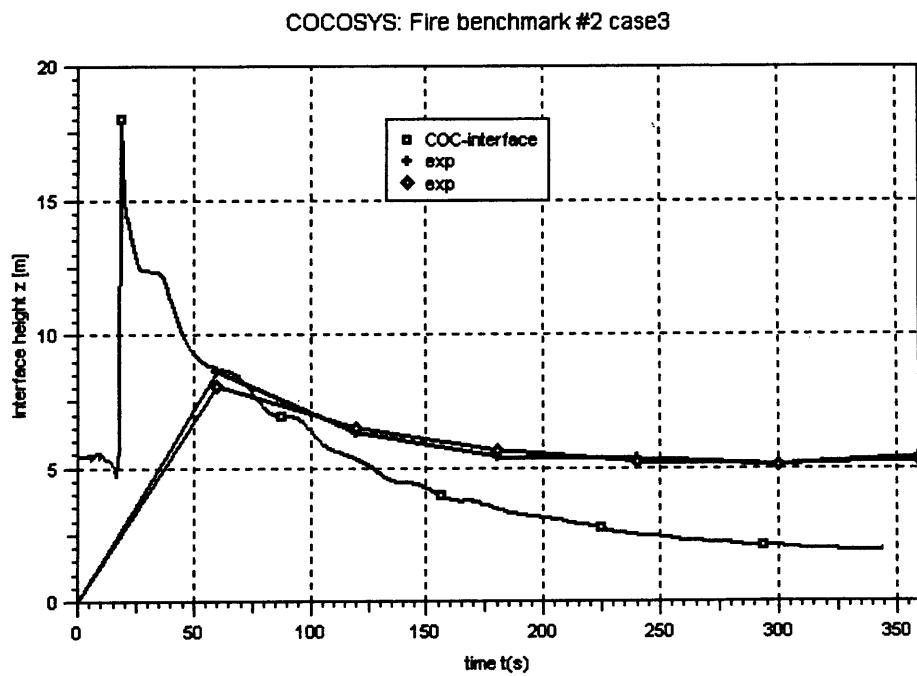


Fig. 3-32 Case 3: Interface height

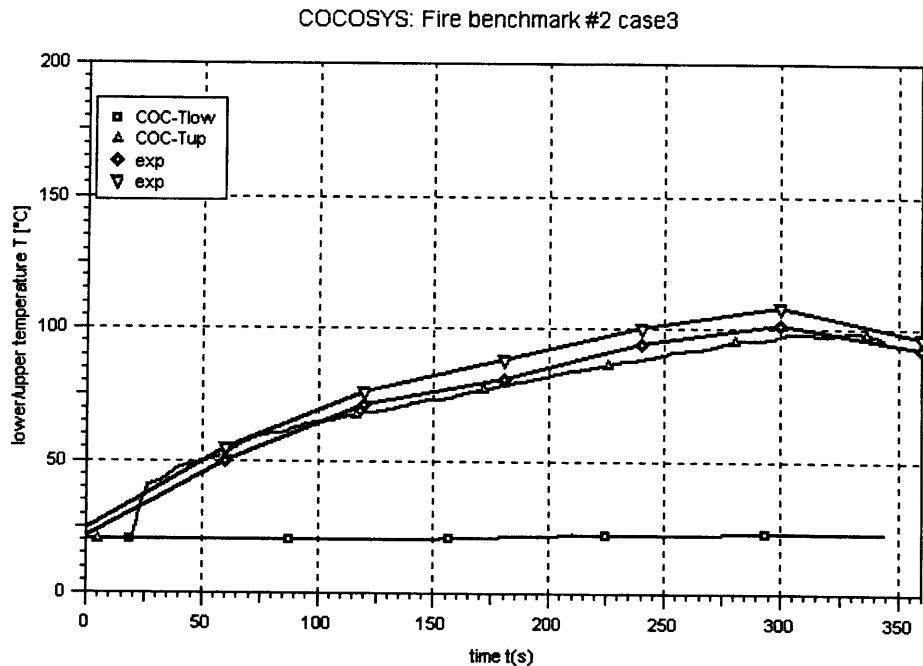


Fig. 3-33 Upper layer temperature

### 3.4 Comparison between the cases

Between the different experiments (case1 to case 3) the experimental boundary conditions have been somewhat changed. From case 1 to 2 the surface of the pool have been increased. And in case 3 the ventilation system has been used and the doors are open. The calculated heat release rates (Fig. 3-34) and temperatures at T1.10 (Fig. 3-35) show a consistent behavior according to the modifications. The increasing of the pool surface leads to an increased heat release rate and increased temperature. Starting the ventilation system (with open doors) lead to a further increase of heat release rate and a reduced burning time. The difference between case 2 and case 3 is relatively small (compared to that between case 1 and 2) because in each case there are oxygen rich conditions. An additional ventilation has only a minor effect in this case.

Although the temperatures are to high, the CFX code delivers consistent behavior too. Fig. 3-36 presents the results of CFX and COCOSYS (*COClfull* variation) in comparison with the experimental data.

COCOSYS: Fire benchmark #2

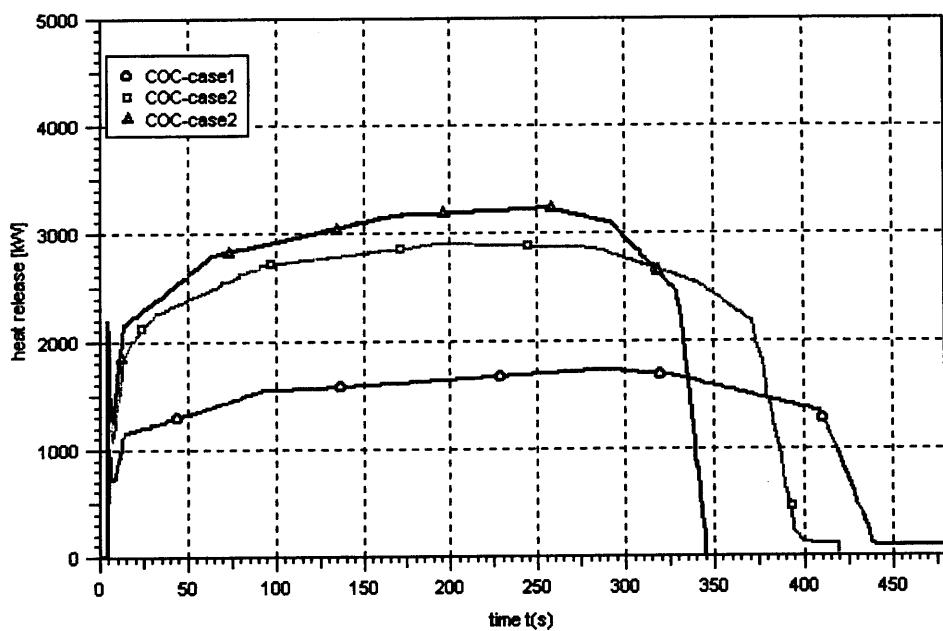


Fig. 3-34 Calculated heat release rates for the 3 cases

COCOSYS: Fire benchmark #2

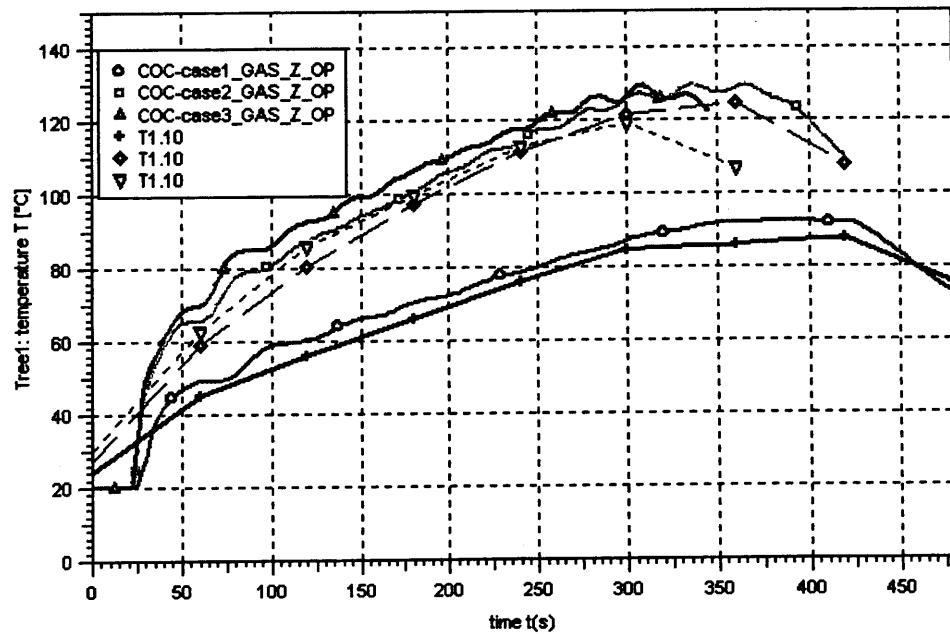


Fig. 3-35 Comparison of the measured and calculated temperatures at T1.10

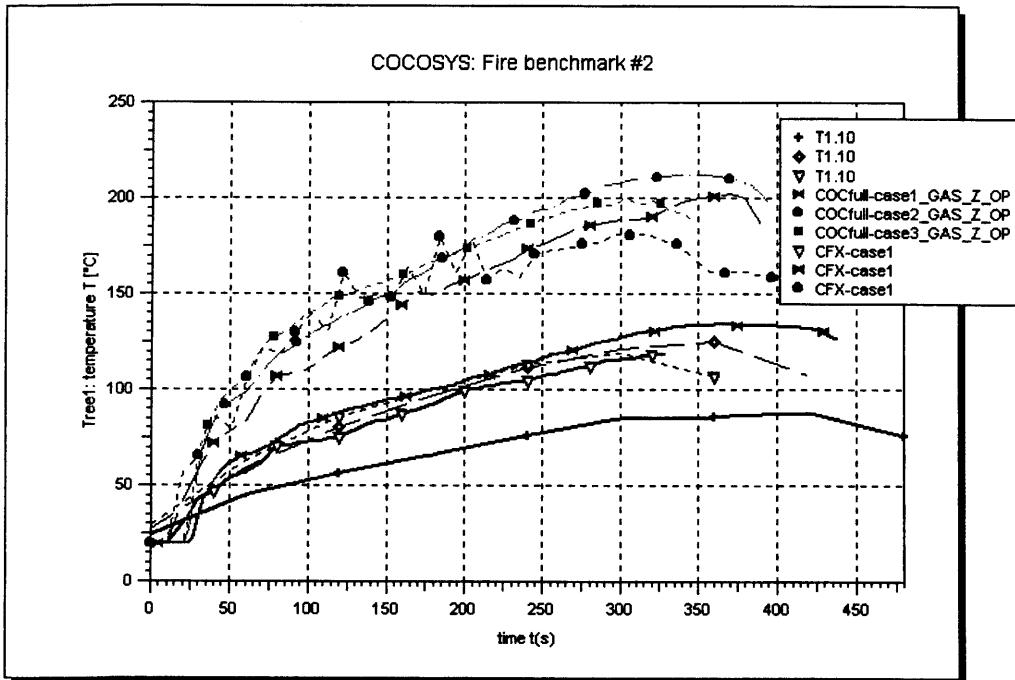


Fig. 3-36 Comparison of CFX and COCOSYS for all cases

#### 4 Conclusions - Next steps

COCOSYS show for the temperature good results in comparison with the experimental data. The calculated temperature stratification in the hot gas layer is somewhat too high. The missing plume model leads to some restriction for the calculated plume temperatures. It has to be pointed out, that the reaction efficiency has been adjusted to the experimental data. The resulting value of about 70 % burned heptan mass seems to be somewhat low. Therefore it would be nice if some more experimental data would be available (concentrations, temperature decrease after burning, velocities). Up to now, COCOSYS has also no model to simulate the soot behavior.

The influence on temperature on different simulation of some boundary conditions (heat transfer to walls, infiltration) leads to a temperature decrease of about 20 K. In comparison to the effect of the efficiency factor this is rather low. One reason may be, that there are oxygen rich conditions, why the differences between case 2 and case 3 are also very small.

The CFX results are delivering too high temperature, corresponding to the initial COCOSYS calculations with complete burning of heptan. Concerning CFX the stability has to be improved (especially for case 3), the infiltration has to be checked. It has already been found, that a reduction of the so-called eddy-break-up-factor would improve the results.

For COCOSYS it is planned to use the detailed model, where the pyrolysis rate is calculated by the program. Therefore some additional initial data is necessary. The efficiency factor should be checked against other experiments.



## **First Results of COCOSYS and CFX Calculations for Benchmark Exercise #2 part 1 Fire in a large Hall**

**Gesellschaft für Anlagen- und Reaktorsicherheit (GRS)mbH**

*International Collaborative Project to Evaluate Fire Models  
for Nuclear Power Plant Applications*

Gaithersburg, May 2-3, 2002

W. Klein-Heßling, M. Heitach (CFX results)



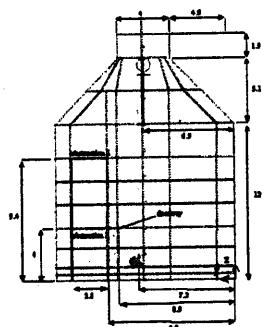
### **Content**

- Nodalisation and used models
- Performed calculations and variations
- First results – special aspects
- Conclusions – next steps

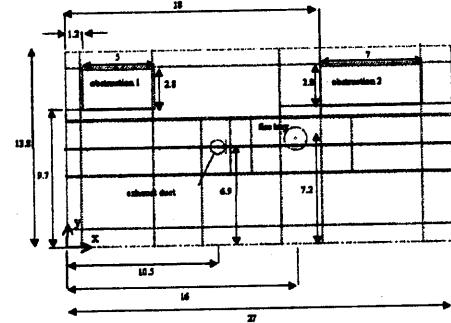
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### COCOSYS Nodallisation

- Side view



- Top view

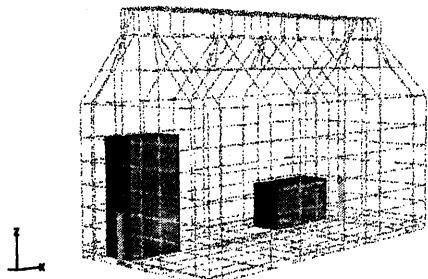


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### COCOSYS Nodallisation (cont.)

- 3D view

Fire benchmark #2  
COCOSYS nodallisation



- Characteristics

- 543 nodes
- 1475 connections
- 421 wall structures

### **COCOSYS Model**

- Pyrolysis model
    - Use of user-defined pyrolysis rate
    - Introduction of a factor for reaction efficiency of 60% above the pool
    - Use of a mixing factor of 2.4
    - Radiation fraction of 20%
  - Radiation
    - Wall-to-wall radiation according specified view factors
    - Distribution of radiated heat (from reaction) according specified view factors from control volumes to wall nodes
- 

### **COCOSYS Model**

- Heat loss through walls
    - 1D-heat conduction model
    - Use of correlations for free convection / or specified value
  - Limitations
    - No plume model
    - No momentum balance
    - No soot model
-

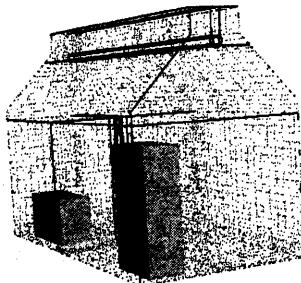
### CFX grid and model

- CFX model

- Use of eddy-break-up combustion model
- Use of Magnussen-soot model
- Use of k-e turbulence model
- Use of radiation model of CFX

- CFX grid

Fire Benchmark #2 part 1  
CFX grid



### Performed calculations - preliminary results

- COCOSYS

- 3 variations for each case
  - full reaction of pyrolyzed heptan (COCfull)
  - reduce efficiency of reaction at surface to 60% (COCbase)
  - change boundary conditions (COCopt)
    - COCOSYS heat transfer models
    - non-adiabatic walls
    - move part of infiltration to top of roof

- CFX

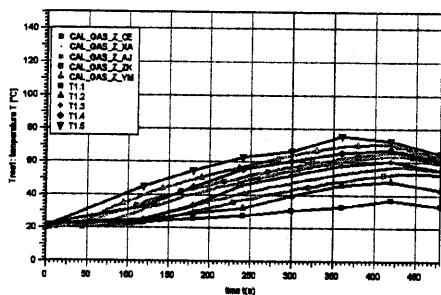
- variation of eddy-break-up rate constant (from 23.5 to 19.)

GRS

### Preliminary results: Case1

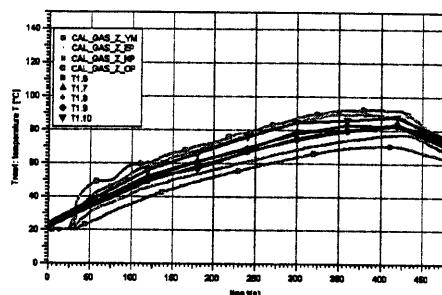
- Tree 1 (lower part)

COCOSYS: Fire benchmark #2 case1



- Tree 1 (upper part)

COCOSYS: Fire benchmark #2 case1

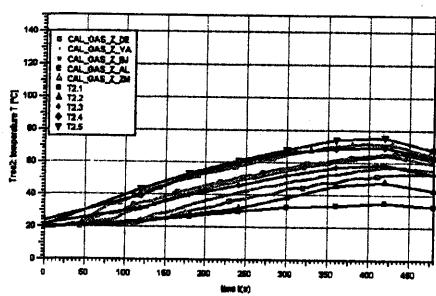


GRS

### Preliminary results: Case1

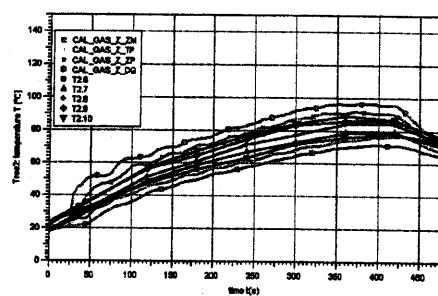
- Tree 2 (lower part)

COCOSYS: Fire benchmark #2 case1



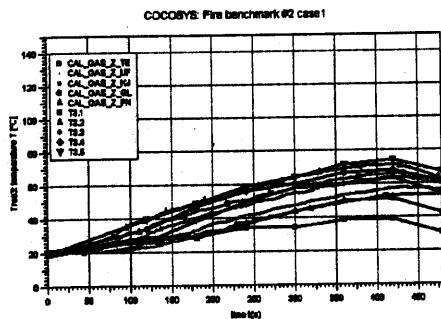
- Tree 2 (upper part)

COCOSYS: Fire benchmark #2 case1

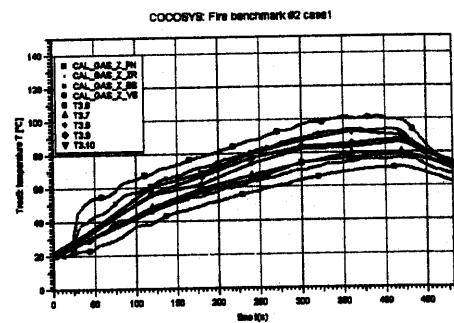


### Preliminary results: Case1

- Tree 2 (lower part)

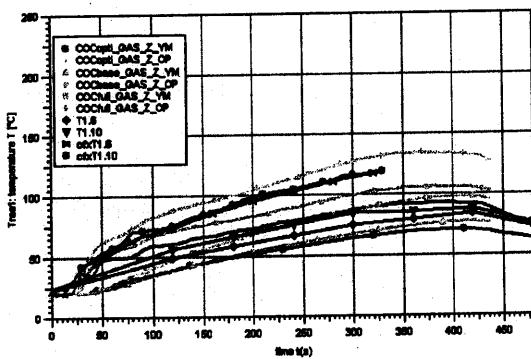


- Tree 2 (upper part)



### Preliminary results: Case1

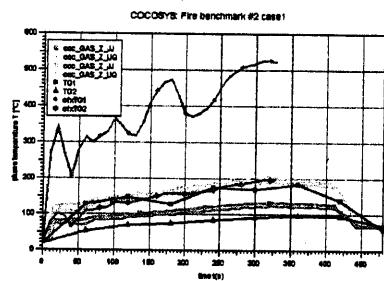
COCOSYS: Fire benchmark #2 case1



- Comparable results for CFX and COCOSYS (variation COCfull)
- Less stratification in CFX according to measurement
- Introduction of local efficiency of 60% leads to good temperatures

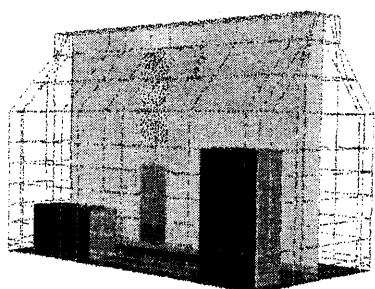
### Preliminary results: Case1

- ,Average' temperatures inside plume
- No plume model in COCOSYS
- Temperatures inside CFX calculations much higher



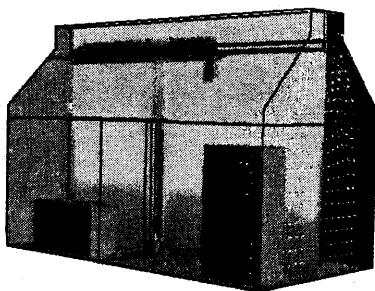
### Preliminary results: Case1

- Plume in COCOSYS  
Fire Benchmark #2 case 1  
COCOSYS calculation



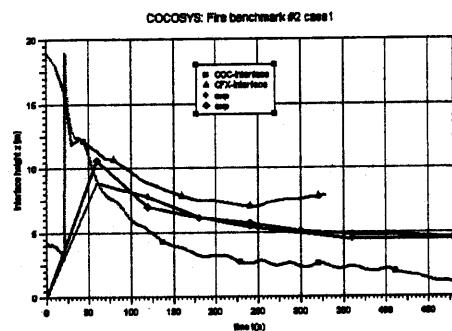
- Plume in CFX

Fire Benchmark #2 part 1  
CFX calculation case1

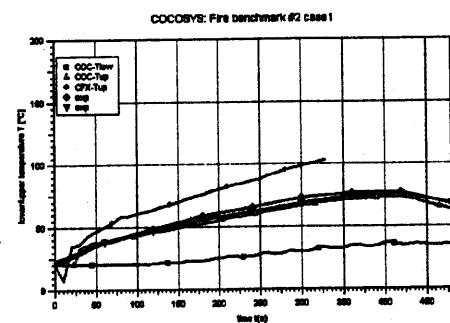


### Preliminary results: Case1

- Interface height

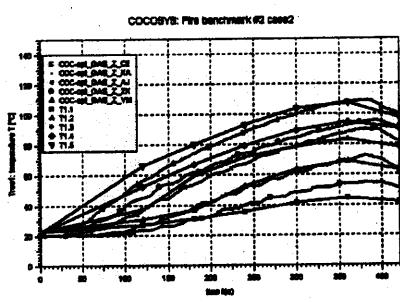


- Upper layer temperature

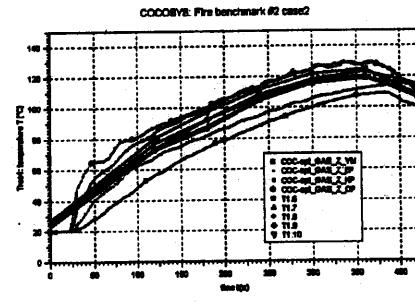


### First results: Case 2

- lower part of tree 1



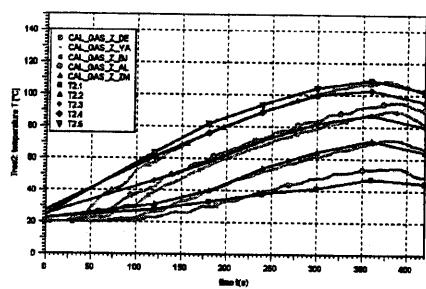
- upper part of tree 1



**First results: Case 2 (cont.)**

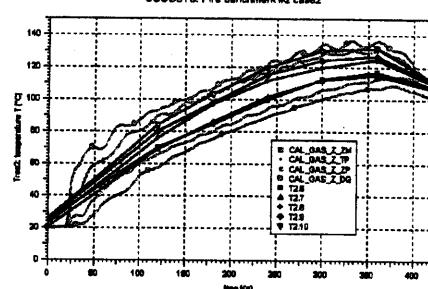
- lower part of tree 2

COCOSYS: Fire benchmark #2 case2



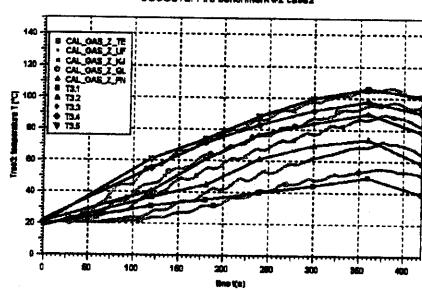
- upper part of tree 2

COCOSYS: Fire benchmark #2 case2

**First results: Case 2 (cont.)**

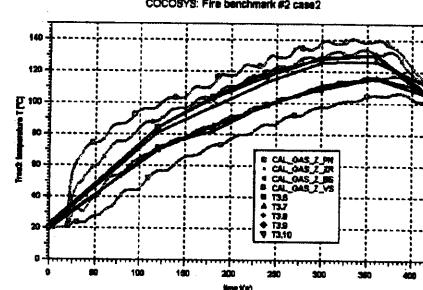
- lower part of tree 3

COCOSYS: Fire benchmark #2 case2



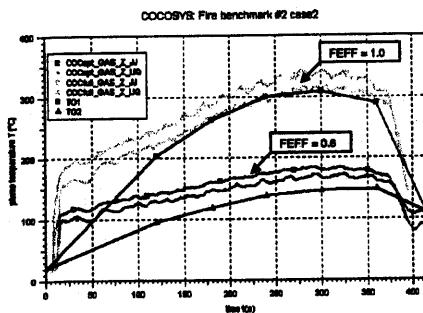
- upper part of tree 3

COCOSYS: Fire benchmark #2 case2

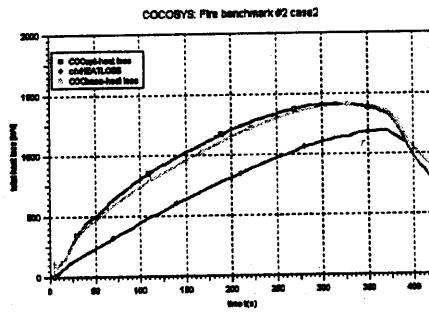


### First results: Case 2 (cont.)

- Plume temperatures

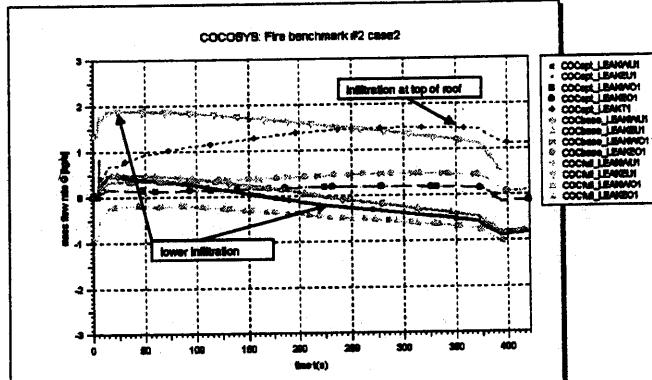


- Heat loss to wall structures



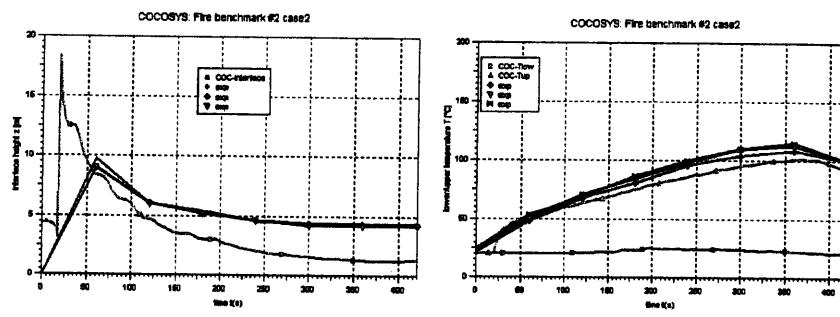
### First results: Case 2 (cont.)

COCOSYS: Fire benchmark #2 case2



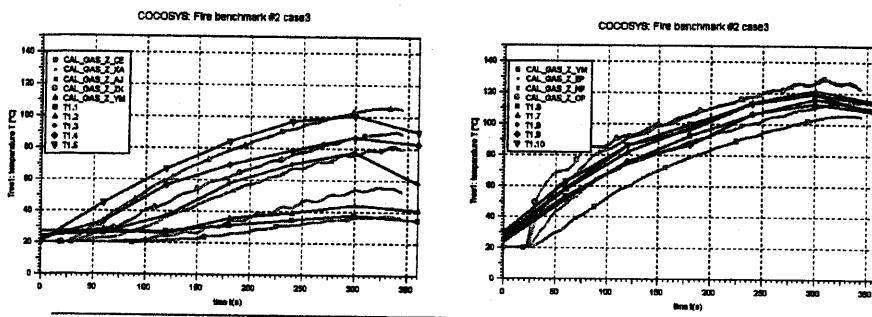
### First results: Case 2 (cont.)

- Height of interface layer
- Upper layer temperature



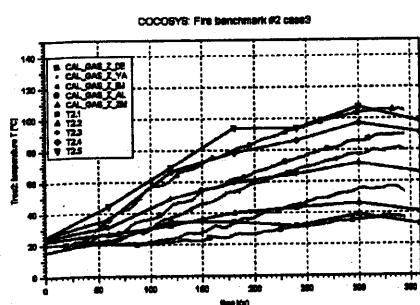
### First results: Case 3

- lower part of tree 1
- upper part of tree 1

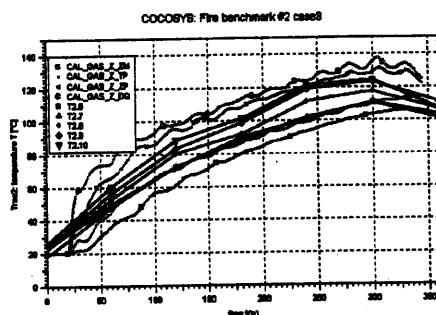


### First results: Case 3 (cont.)

- lower part of tree 2

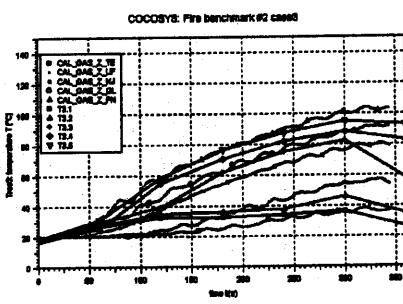


- upper part of tree 2

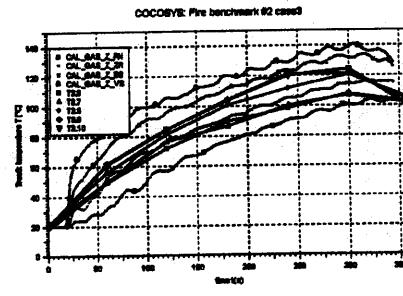


### First results: Case 3 (cont.)

- lower part of tree 3

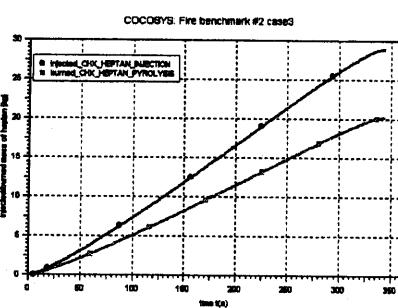
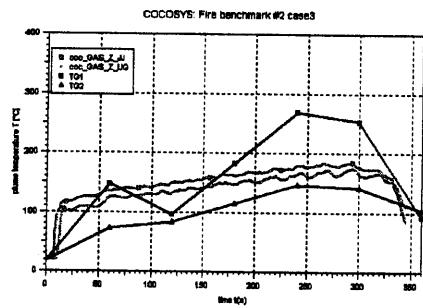


- upper part of tree 3



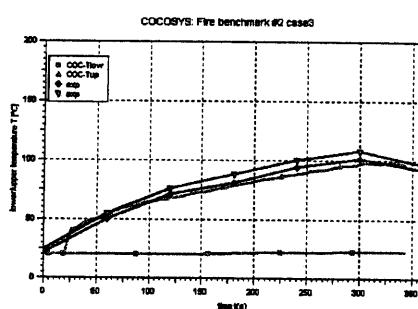
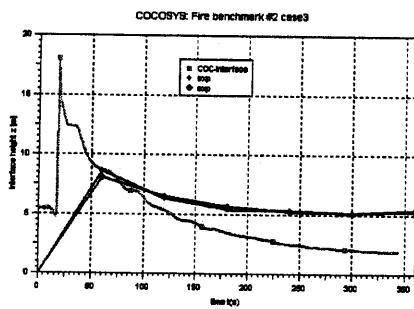
### First results: Case 3 (cont.)

- Plume temperature
- Injected/burned heptan mass  
(about 70% is burned)



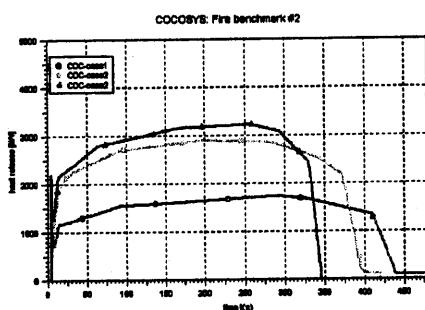
### First results: Case 3 (cont.)

- Height of interface layer
- Upper layer temperature

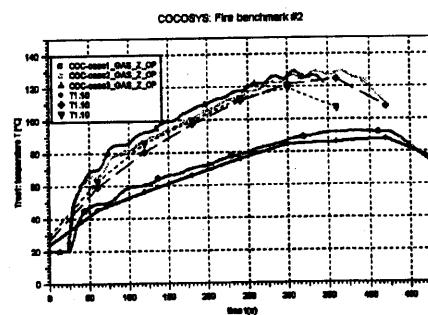


### Comparison between the cases

- Heat release

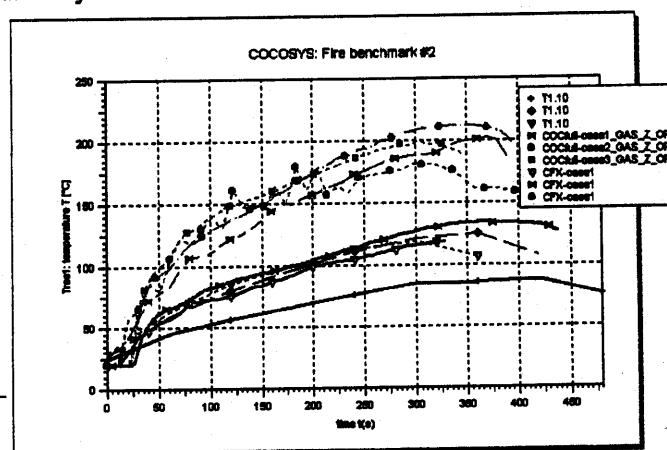


- Temperature (Tree 1 top position)



### Comparison between the cases (cont.)

- Preliminary CFX results and COCOSYS results with complete reaction



### Conclusions – next steps

- COCOSYS
  - Temperature results
    - good results after introducing reactions efficiency of 60% above the pool
    - to strong stratification in the hot gas layer
    - no plume model ( $\rightarrow$  temperature behavior TG1, TG2)
  - Additional experimental data available?
    - Temperature decrease (to check heat loss)
    - Concentration measurements

### Conclusions – next steps (cont.)

- COCOSYS (cont.)
  - Infiltration position/heat loss to walls
    - only small effects on the results
    - care have to be taken for the definition of boundary conditions (environment pressure)
- CFX
  - too high temperatures (similar to COCOSYS results with full reaction)  
 $\rightarrow$  variation of eddy-break-up rate constant
  - hot gas layer temperature homogeneous mixed (as measured)
  - still some problems with boundary conditions

### **Conclusions – next steps (cont.)**

- **Next steps**

- Continue with CFX calculations
  - Use of detailed oil burning model in COCOSYS
    - some more initial data is necessary (oil + water mass, geometry)
  - Additional tests against other experiments